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*Highlights (for review)

- Model as a Service (MaaS) with expert knowledge is proposed as a new architecture of cloud computing.
- A numerical model which simulates the groundwater system is constructed as a case study for the MaaS.
- The parameters in the numerical model are analyzed using sequential data assimilation.
- A first implementation of the MaaS is conducted on the private cloud to prove the feasibility of the architecture.

Integration of numerical model and cloud computing

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Abstract

With the significant advancements in Information and Communications Technology (ICT), cloud based applications provide a novel approach to access applications which are not installed on the local computers. The integration of cloud computing and Internet of Things (IoT) indicated a bright future of the Internet. In this paper, a new architecture of cloud computing—Model as a Service (MaaS) is proposed. The feasibility of the proposed architecture is proved by implementing a groundwater model on cloud as a case study. The groundwater model is established using MODFLOW for the middle reach of the Heihe River Basin (HRB). The model is calibrated using in situ observation to ensure capability of simulating the groundwater process with Root Mean Square Error (RMSE) of 1.70 m and coefficient of determination (R^2) of 0.64. The parameter uncertainties of the groundwater model are analyzed by sequential data assimilation algorithms (PF, Particle Filter; EnKF, Ensemble Kalman Filter) in a synthetic case. The results show that the parameter uncertainties are effectively reduced by incorporating observed information recursively. A comparison between PF and EnKF indicate that the results from PF are slightly better than those from EnKF. The integration shows a bright future for simulating the groundwater system in real-time. This study provides a flexible and effective approach for analyzing the uncertainties and time variant properties of the parameters and the proposed architecture of cloud computing provides a novel approach for the researchers and decision-makers to construct numerical models and follow-up researches.

Keywords: Cloud computing; Numerical model; Model as a Service

1. Introduction

Numerical models have been widely used in the mathematical modeling of many natural systems (e.g., hydrology, climatology, biology, physics, chemistry) and human systems (e.g., economics, social science and engineering) with the ability to explore and investigate the natural systems. However, scientific computing is a victim of its own success in some ways. Researchers tend to develop complex models to involve various processes, data sources, management alternatives and analysis algorithms. Significant computational resource and time are required while constructing the complex models which would distract the researchers from their research interests. Moreover, the reusability of numerical models between different research groups is limited which lead to significant waste of resources. A new architecture which makes use of all the endeavors toward numerical models would be great help. In this paper, groundwater model was selected to address the issues. Groundwater models simulate the spatiotemporal variability of the groundwater system in the aquifers and bridge the gap between field observations and general characterization of the whole system. In general, groundwater models are implemented by applying finite-difference or finite-element approximations and use distributed parameters which are not directly measured and have to be determined from calibrations. The desire for solving larger, more sophisticated groundwater problems requires improvements to scientific methodology, algorithms and temporal-spatial resolutions which are always accompanied by increases in the complexity of the groundwater models.

With the rapid development in Information and Communications Technology (ICT), cloud computing has emerged as a new paradigm for sharing the configurable computing resources (e.g., servers, applications, storage, services and computer networks) [1, 2]. The computing resources are becoming important as computing being transformed to the 5th utility (after water, electricity, gas and telephony) [3]. Fortunately, the rapid development of processing and storage technologies and the success of the Internet, the computing resources are becoming more powerful, cheaper and ubiquitously available than ever before which leads to the cloud computing. Following the results of the evolution and adoption of existing technologies and paradigms, cloud computing enables the users access the infrastructure, platform and software as a service. In a cloud computing environment, there are four standard models those are Infrastructure as a Service (IaaS), Platform as a Service (PaaS), Software as a Service (SaaS) and Data as a service (DaaS) [1, 4]. In the SaaS model, cloud providers install, operate and manage software in the cloud and users gain access to software and databases from cloud clients. SaaS offers high scalability which provides users the option to access more or fewer service or features on-demand. Another important technology—Wireless Sensor Networks (WSNs)—bridged the gap between the cyber world and the physical world and led to cyber-physical systems (CPSs). The main reason for the development and evolution of CPSs are to intelligently monitor and control our physical world and the requirements for reducing the development costs and time and enhancing the designed products. Although the cloud computing and WSNs had experienced a rapid evolution independently and were different from each other, their characteristics were often complementary [5]. Therefore, the integration of cloud computing and WSNs were proposed by many researchers in order to benefit from both technologies [5-7].

The complication of the groundwater models usually leads to the increase of parameters which maintained the consistency between the simulated system behavior and the corresponding observations [8]. Many techniques had been developed to determine the parameters of numerical models. Traditionally, the parameters were determined based on trial-and-error adjustments and visual inspection of the agreements and differences between the simulations and observations for some historical records [9, 10]. The automatic parameter estimation techniques had been motivated by the subjectivity and time-consuming nature of trial-and-error adjustments [11-15]. However, these methods always lack the capability to properly take into account various uncertainties inherent in the system and easily stuck in the local minimum. Sequential data assimilation techniques provide a general framework for automatic parameter estimation and at the mean time explicitly considering the uncertainties from the inputs, parameters and model structures. One of the most well-known data assimilation algorithm based on recursive Bayesian estimation techniques was the Kalman Filter (KF) [16]. However, KF was only applicable to linear systems. The Extended Kalman Filter (EKF) was then developed for optimizing nonlinear systems [17]. The major drawback of the EKF is the requirement to linearize the model equations which lead to notoriously inaccuracy if the nonlinearities are strong. The well-known ensemble Kalman-filter (EnKF) [18], a Monte Carlo implementation of Bayesian updating was proposed by Evensen to circumvent the problems by evolving the errors with the nonlinear model by performing an ensemble of model runs. However, EnKF relies on a Gaussian assumption of model and observation errors which is not always true in environmental modeling [19-21]. In a separate research line, the use of sequential Monte Carlo methods in the form of PF [22, 23] for non-Gaussian, non-linear dynamical models had been developed [22, 24, 25]. The PF originated from the research area of target tracking, object recognition, robotics and financial analysis. The advantage of PF is the handling of non-Gaussian, non-linear models. Both PF and EnKF use samples (i.e., ensemble members in EnKF, particles in PF) to estimate the Probability Density Function (PDF) of model states and parameters.

Groundwater plays a valuable role in the agricultural production, economic development and ecological balance in the middle reaches of the Heihe River Basin (HRB). Owing to several unique qualities (e.g., widespread and continuous availability, low development cost, drought reliability, etc.), groundwater has been excessively exploited during the last decades. Groundwater over-exploitation would cause many impacts which include groundwater level drawdown, reduced streamflow, increased energy cost for pumping, deterioration of water quality and ecological degradation [26]. Groundwater models are widely used methodology to parameterize the geologic structure of the real world. Many groundwater models had been developed in the last three decades [27-31]. MODFLOW [30], a well-established US Geological Survey computer software had been widely used to simulate groundwater system since the early 1990s.

The core contributions of this study were (1) the simulation of groundwater system in the middle reaches of the HRB, (2) the estimation of parameters and parameters uncertainties, (3) a new architecture of cloud computing based on Software as a Service (SaaS) which leads to the concept of Model as a Service (MaaS). We will first outline the theory behind the cloud computing, SaaS, PF and the groundwater model. This will be followed by the descriptions of data source and model settings. Section 4 and section 5 will present the results and conclusions.

2. Related works

Although the origin of the term “cloud computing” in ICT is unclear, the idea of cloud computing is not new. In the Fall of 1957, Professor John McCarthy tried to initiate time-sharing on modified IBM 704 and IBM 7090 computers [32]. Later in 1961, he first suggested a vague model of computer time-sharing system which was regard as the early stage of cloud computing [33]. The National Institute of Standard and Technologies (NIST) provided the definition and reported several essential aspects of cloud computing [34]. Several architectures of cloud computing were proposed by [1, 35, 36] which were Infrastructure as a Service (IaaS), Platform as a Service (PaaS), Software as a Service (SaaS), Data as a service (DaaS) and Robot as a Service (RaaS). The architectures, interfaces, and behaviors of intelligent devices connected to the cloud computing environment were discussed using RaaS as a case study [37]. All these architectures lead to Everything as a Service (EaaS, XaaS or *aaS) [38] (Fig. 1). An extensive survey of mobile cloud computing was given by [39]. Recent research advances of applications of cloud computing techniques in scientific research were reviewed by [40]. Dong et al. reported a novel evacuation system based on multiple cloud platforms in order to provide better management with lowers costs in an emergency [41]. More recently, Tao et al. proposed a hybrid computing model named “Foud” which combined fog computing and cloud computing to optimize Vehicle-To-Grid network services [42]. CPS extends the cloud computing concept beyond computing and communication to include physical devices [37]. CPSs require tight integration of computing, communication and control technologies in managing physical systems and applications [43]. A comprehensive survey on the concept and strategies for constructing resilient and integrated CPSs was given by [44, 45]. The pervasiveness of WSNs technologies in many fields makes them an integral part of CPSs [46]. Several issues related to WSNs were addressed by the scientific community [47]. The risk assessment and security issues in CPSs were studied by [48-54]. Several examples based CPS were described by [55-57].

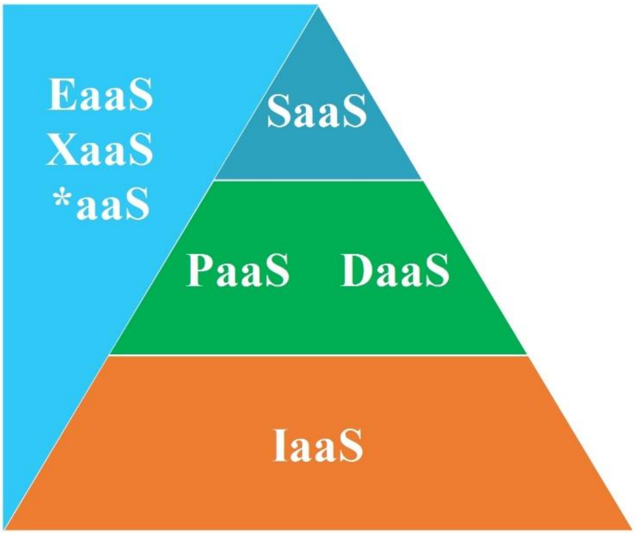

Fig. 1. The Architectures of Cloud Computing.

Particle Filter was used to solve nonlinear filtering and Hidden Markov Chain (HMM) problem in Bayesian statistical inference and signal processing which was pioneered by [22]. The mathematical foundations and the first rigorous analysis of the PF was described by [58, 59]. Some branching types of particle methodologies were developed in the 1990s [60, 61]. The sample degeneracy and impoverishment problem in PF were investigated by [62]. Bi et al. developed an improved PF and tested it by assimilating temperatures into the variance infiltration capacity (VIC) model to estimate soil moisture in the NaQu network region at the Tibetan Plateau

[63]. Salamon et al. applied the PF to assess parameter, precipitation, and predictive uncertainty in the rainfall–runoff model LISFLOOD and explored the capabilities of PF for handling the parameter uncertainties [64]. Hongxiang Yan and Hamid Moradkhani reported a study which assimilated streamflow and surface soil moisture into Sacramento Soil Moisture Accounting (SAC-SMA) model using PF. Albrecht H. Weerts and Ghada Y. H. El Serafy compared PF and EnKF in updating the state in a conceptual rainfall-runoff model HBV-96 for flood forecasting and concluded that PF performed better than EnKF for estimating the soil moisture storage states with little difference [65].

Many numerical models have been developed for hydrological systems over the last 30 years [28, 30, 66-68]. These numerical models provided effective approaches to simulate and analyze the spatial–temporal variations in the distribution of groundwater system under changing land use and climate conditions, and hence, analyze the hydrological responses to different climate and land use scenarios. Many researches had been conducted using the hydrological models [69-77].

3. Materials and Methods

3.1 Model description

In this paper, the framework of integrating cloud computing and WSNs was used followed [5, 56]. WSNs deployed in the physical world were used to gather data from the environment for the cloud computing as illustrated in Fig. 2. Several modifications were made based on the Berkeley view of cloud computing [78] which led to the new architecture Model as a Service (MaaS). Fig. 2 illustrated four layers (including MaaS Users in the top layer) in the proposed architecture. The bottom layer contained the physical machines which provided the computing resources (e.g., CPU, Memory, Disk, Bandwidth, etc.). The second layer mediated and managed the physical resources. Virtual machines ran on the hardware resources which were considered as a perfect method to overcome the establishment and maintenance of physical machines. The idea of virtualization of the computing resources includes processors, memory, disk and I/O devices aiming to improve sharing and utilization of the computing resources [79-82]. Virtualization enables multiple and different operating systems and softwares to operate on a single physical platform (IaaS). The third layer was the numerical model layer. Numerical models are usually computer programs which can simulate the behaviors, dynamics of natural systems in physics, astrophysics, climatology, chemistry and biology, human systems in economics, psychology, social science, and engineering [83]. They can be used to explore, capture and reproduce the performance of natural systems which are too complex for analytical solutions [84]. Different kinds of numerical models (e.g., groundwater models, subsurface models, land surface models, climate models, etc.) could be established on the virtual machines. Models were supposed to construct and calibrate offline with extensive expert knowledge according to different purpose and offered as a service (MaaS) so that the users could focus on their principal problems. Theoretically, these models were distributed in different locations and could be accessed via Internet. Moreover, three fundamental requirements of Service-Oriented Architecture (SOA) [85] functions should be satisfied as a service provider, as a service broker and as a service client:

- **As a service provider:** A repository of preloaded services (e.g., models and components) is provided. The information of the services is also hosted and provided to the service broker. MaaS users (e.g., researchers and modelers, etc.) can deploy new services into or remove service from a model.

- **As a service broker:** A list and information of the services which are available are provided to the MaaS users.
- **As a service client:** MaaS users are able to compose new models based on the services available. The entries in the broker registry for the selected services are located using various find operations.

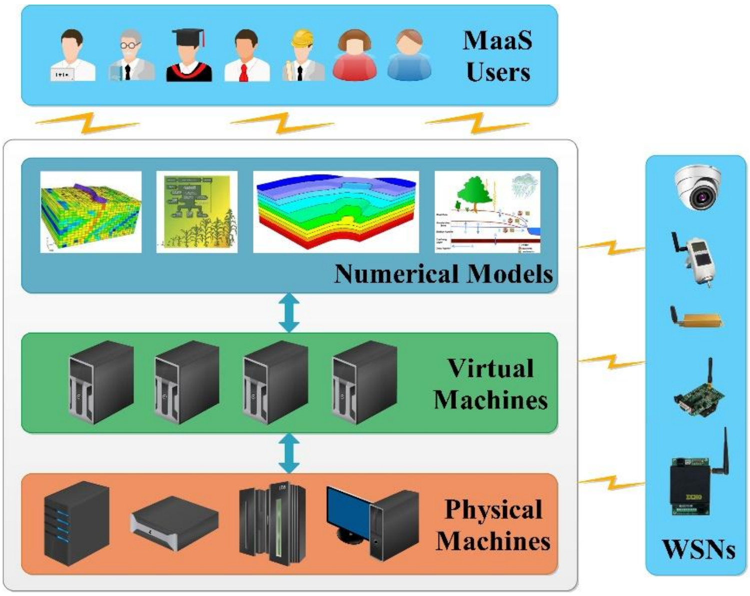

Fig. 2. Architecture of Model as a Service

3.2 Particle Filter

Particle Filters [86] allows inference of full posterior distributions via Bayesian filtering in nonlinear state-space of models with non-Gaussian noises. With sufficient samples, the particles would approach the Bayesian optimal estimate. A brief introduction of PF is given below.

3.2.1 Recursive Bayesian Estimation

The central idea of PF is to represent the PDF of model states as a set of random samples.

The state vector evolves according to

$$X_n = M\left(X_{n-1}, \theta, u_{n-1}\right) + V_n \tag{1}$$

Where $M(\bullet)$ is the system transition function which normally is a model and V_n represents the system noise. X_{n-1} is the state variables at time step n-1. θ represents the vector of model parameters. At discrete times, the measurement Y_n would be available. The states transform to the measurement domain using the observation equation.

$$Y_n = H\left(X_n, \theta\right) + U_n \tag{2}$$

Where H is the observation operator which expresses the transition from states to the measurements and U_n is the measurement noise. The noise terms of V_n and U_n are generally assumed to be independent random vectors. On time step n, the available information of measurements is $D_n=\{Y_n;\ n=1, 2, \ldots, t\}$.

The purpose is to acquire the PDF of the current state given all the available information $p(X_n|D_n)$. This PDF can be obtained recursively in two procedures: prediction and update. Suppose that the PDF $p(X_{n-1}|D_{n-1})$ at time step n-1 is available. For the prediction stage, the prior PDF of the state at time step n is:

$$p\left(X_n \mid D_{n-1}\right)=\int p\left(X_n \mid X_{n-1}\right) p\left(X_{n-1} \mid D_{n-1}\right) dX_{n-1} \tag{3}$$

After the Y_n becomes available at time n, the posterior PDF could be obtained via Bayes rule (the update stage):

$$p\left(X_n \mid D_n\right)=\frac{p\left(Y_n \mid X_n\right)\mathrm{p}\left(X_n \mid D_{n-1}\right)}{p\left(Y_n \mid D_{n-1}\right)} \tag{4}$$

Where the normalizing constant is given by

$$p\left(Y_n \mid D_{n-1}\right)=\int p\left(Y_n \mid X_n\right) p\left(X_n \mid D_{n-1}\right) dX_n \tag{5}$$

In equation (4), Y_n (the measurements at time step n) is used to update the prior PDF for time step n-1. The recurrence of equation (3) and (4) along time step is the formal solution to Bayesian estimation problem.

3.2.2 Sequential importance sampling (SIS)

In PF, the posterior distributions are approximated by discrete random measures implemented by particles and the associated weights. The particles at time step n are used to map integrals to discrete sums by the following approximation [24]:

$$p\left(X_{0:n} \mid Y_{1:n}\right) \approx \sum_{i=1}^{N_p} w_n^i \delta\left(X_{0:n}-X_{0:n}^i\right) \tag{6}$$

Where $\{X_n^i, w_n^i\}$ represents the ith particle at time step n and its weight, respectively. The weights w_n^i sum to 1. δ(•) denotes the Direc delta function.

An important concept in PF is the SIS which is used for the determination of the particle weights [87]. The importance sampling generates particles X_n^i from a proposal distribution (or importance density) $q(X_{0:n}|D_{1:n})$ and assigns the weights (importance weights) according to

$$w_n^i \propto \frac{p\left(X_{0:n}^i \mid D_{1:n}\right)}{q\left(X_{0:n}^i \mid D_{1:n}\right)} \tag{7}$$

The update of the importance weights at iteration is achieved by factorizing the proposal distribution sequentially [24, 25]:

$$w_n^i = w_{n-1}^i \frac{p\left(Y_n \mid X_n^i\right) p\left(X_n^i \mid X_{n-1}^i\right)}{q\left(X_n^i \mid X_{0:n-1}, Y_{1:n}\right)} \tag{8}$$

The SIS algorithm has serious degeneracy limitations [25]. To surmount this limitation, a resampling stage needs to be introduced which will be briefly presented in the following section.

3.2.3 Sequential importance resampling (SIR)

The SIR eliminates samples with low weights and accumulates samples with high importance weights by mapping the Dirac random measure $\{X_{n-1}^i, w_{n-1}^i\}$ into an equally weighted random measure $\{X_{n-1}^i, 1/N_p\}$ so that N_p particles are produced all with weighting $1/N_p$.

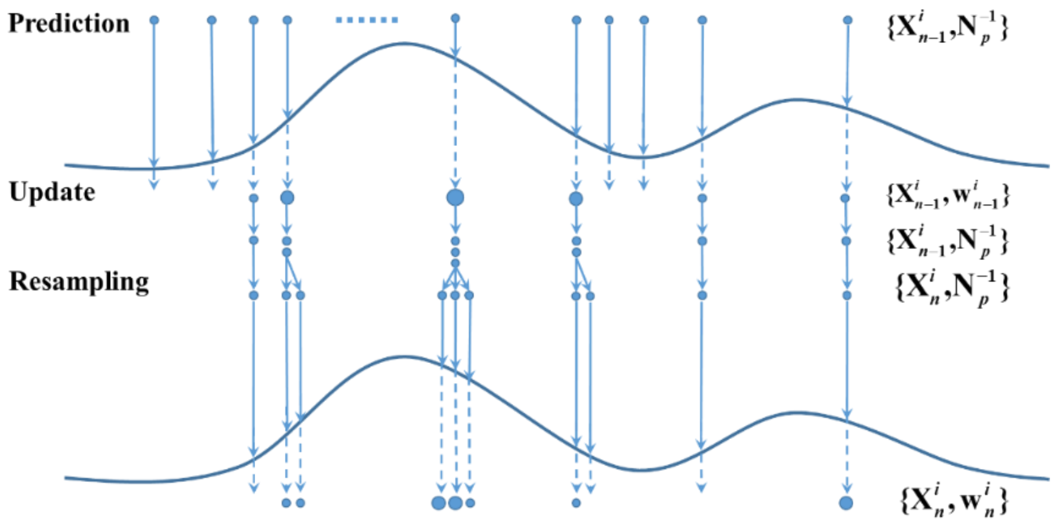

Fig. 3. Schematic diagram of Particle Filter

As shown in Fig. 3, the PF starts at time step n-1 with a uniform distributed measurements $\left\{X^i_{n-1}, N^{-1}_p\right\}$ which provides an approximation of $p(X_{n-1}|D_{1:n-2})$. The importance weights for particles are computed at time step n-1. This results in the weighted measure $\left\{X^i_{n-1}, w^i_{n-1}\right\}$ which provides an approximation of $p(X_{n-1}|D_{1:n-1})$. The resampling step selects only the fittest particles to obtain the unweighted measure $\{X^i_n, N^{-1}_p\}$ which is also an approximation of $p(X_{n-1}|D_{1:n-1})$. Finally, the prediction step introduces variety in the measure of the next time step $\{X^i_n, N^{-1}_p\}$ which yields an approximation of $p(X_n|D_{1:n-1})$.

3.3 Numerical model

In this study, the numerical model MODFLOW [30] was used to simulate the groundwater flow. MODFLOW numerically solves the three-dimensional groundwater flow equations using a finite-difference method.

$$\frac{\partial}{\partial x}\left(K_{xx}\frac{\partial H}{\partial x}\right)+\frac{\partial}{\partial y}\left(K_{yy}\frac{\partial H}{\partial y}\right)+\frac{\partial}{\partial z}\left(K_{zz}\frac{\partial H}{\partial z}\right)-W=S_s\frac{\partial H}{\partial t} \tag{9}$$

Where H is the hydraulic head (L); K_{xx}, K_{yy}, K_{zz}, are values of hydraulic conductivity along the x, y and z coordinate axes (L/T); W represents source and/or sink term of water (T^{-1}) with $W < 0$ for flowing out of the groundwater system, and $W > 0$ for flowing into the system; S_s denotes the specific storage of the aquifer (L^{-1}); and t is time(T).

3.4 Data and model settings

Land use data were obtained through interpretation of Landsat TM/ETM+ images in [88-90] which was developed by the Chinese Academy of Sciences (CAS). Observed groundwater level data from 42 boreholes (Fig. 4 (a)) were used in for calibrating the model. The irrigation data were obtained from annual water resource management reports published by the Zhangye Municipal Bureau of Water Conservancy. Annual runoff at Yingluo Gorge, Gaoya and Zhengyi Gorge hydrologic stations (Fig. 4 (a)) were collected from the Gansu Provincial Bureau of Hydrology. The data of groundwater exploitation during the modeling period were obtained from China

Census for Water. All of the above-mentioned data were collected by WSNs and obtained from the Environmental and Ecological Science Data Center for West China (WestDC, http://westdc.westgis.ac.cn/).

The construction of conceptual model for the middle reaches of the HRB was shown in Fig. 5. From the perspective of the whole middle reaches, there are several source and sink terms. These terms can be summarized as follows:

$$Irr + Q_{Liyuan} + Q_{Heihe} + Q_{Bou} - ET - Q_{Heihe} = \Delta Storage \tag{10}$$

Where *Irr* is the irrigation for the farmland (L/T); Q_{Liyuan} is the inflow of the Liyuan river (L^3/T); $\underline{Q_{Heihe}}$ is the inflow of the Heihe river from the upper reaches which is observed at Yingluo hydrologic station (L^3/T); Q_{Bou} is the inflow from system boundary (L^3/T); *ET* is evapotranspiration (L/T); Q_{Heihe} represents the outflow to the lower reaches which is observed at Zhengyi Gorge hydrologic station (L^3/T); $\Delta Storage$ is the variation of the groundwater storage in the middle reaches. Constant flux boundary is defined for the south and east boundary where groundwater flows into the model domain from mountains; the north side of the middle reaches is the impermeable boundary; impermeable boundary is selected at the tectonic fault-down zone in the west; the top boundary is atmospheric air-soil interface; the bottom boundary condition at the base of aquifer is defined as no-flow boundary.

MODFLOW was used to simulate the groundwater dynamics in the middle reaches of the HRB [91] (Fig. 4 (a)). The middle reaches of the HRB was conceptualized by finite-difference grids which consisted of 132 rows and 165 columns with a uniform cell size of 1×1 km (Fig. 4 (b)). The simulation was conducted from January 1986 to December 2008 with 276 stress periods. The agricultural irrigation was simulated through Recharge (RCH) package [30] in MODFLOW-2005 by specifying recharge flux during the study periods. Evapotranspiration was simulated using the Evapotranspiration (EVT) package [30]. Groundwater discharge from evapotranspiration was neglected when the groundwater level is lower than 5 m. There were over 6000 pumping wells in the study area; however, 805 pumping wells were simulated in MODFLOW due to the resolution of model grids (Fig. 4. (b)). The Heihe River and Liyuan River was implemented using the Streamflow-Routing (STR) package [92] (Fig. 4. (b)). The study area was divided into eight sub-zones according to hydrogeological map [93]. The horizontal hydraulic conductivity (parameters) were constant for each sub-zone (Fig. 6).

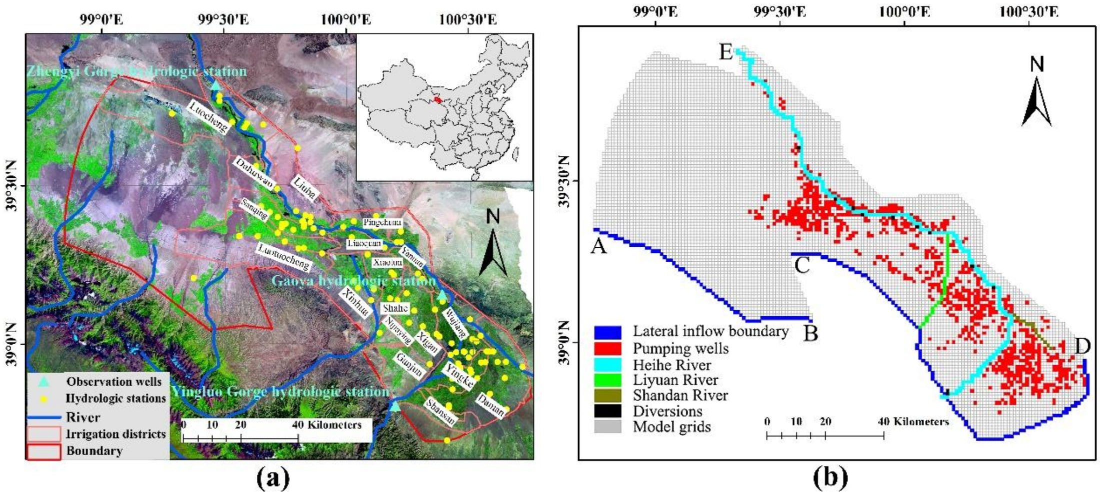

Fig. 4. (a) Location and map of the middle reaches of the Heihe River Basin; (b)

Conceptualization of the middle reaches of the Heihe River Basin in MODFLOW

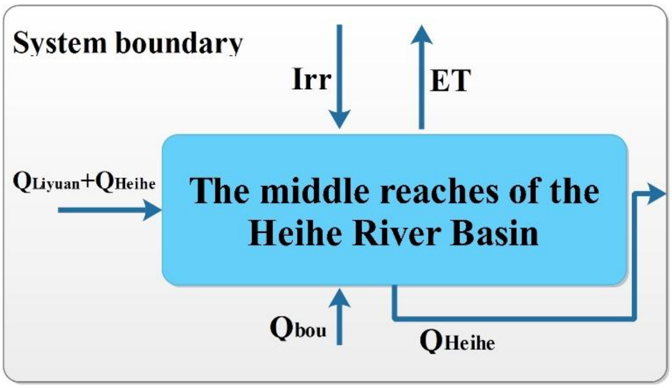

Fig. 5. Conceptual model for the middle reaches of the Heihe River Basin

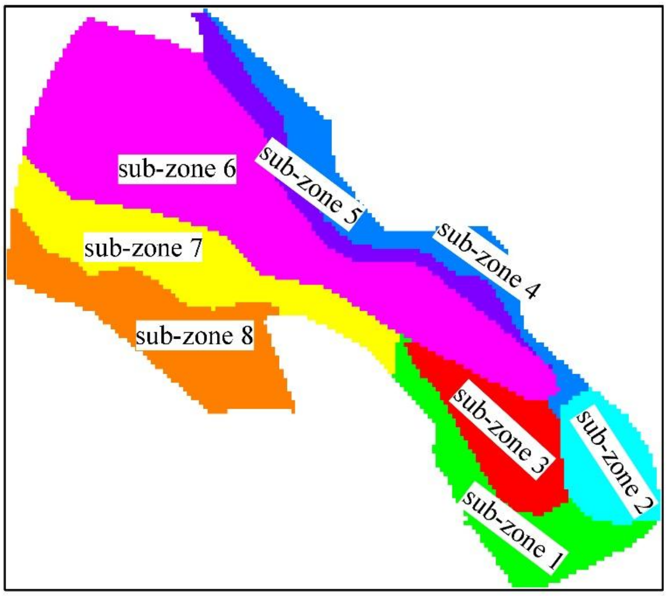

Fig. 6. The subzones of hydraulic conductivity in the middle reaches of the Heihe River Basin

4. Results and Analysis

4.1 Groundwater level simulation

Seven boreholes (one for each sub-zones of hydraulic conductivity) were selected from the 42 wells to illustrate comparisons of the observed and simulated groundwater level (Fig. 7). No comparisons were conducted in sub-zone 8 because of the absence of observed data. The model parameters were calibrated in the middle reaches of HRB using different types of data. The calibration was accomplished by a combination procedure of the parameter estimation code PEST [94] and trial-and-error. The calibration makes the simulated results to approximate the measured data from the boreholes as much as possible. Through this process, the model parameters (hydraulic conductivity) were adjusted and shown in Table 1. The observed and simulated groundwater level at all the observation wells in the calibration period (Fig. 7 (h)) indicated a reasonable match between the observed and simulated head values. A quantitative comparison of the head data in all observation wells was carried out to evaluate the model performance with RMSE of 1.70 m and R^2 of 0.64. The discrepancy was reasonable considering the inaccurate spatial distribution of the initial hydraulic heads and the relatively large difference between the highest and lowest groundwater level across the model domain with about 230 m. However, from Fig.7 (a) to Fig. 7 (g) one could notice that there were still some differences between the observed and simulated groundwater levels.

Table 1

Calibrated hydraulic conductivities for each sub-zone

Sub-zones / Parameters	1	2	3	4	5	6	7	8
Hydraulic conductivities (m/day)	23	10	90	3	20	20	50	50

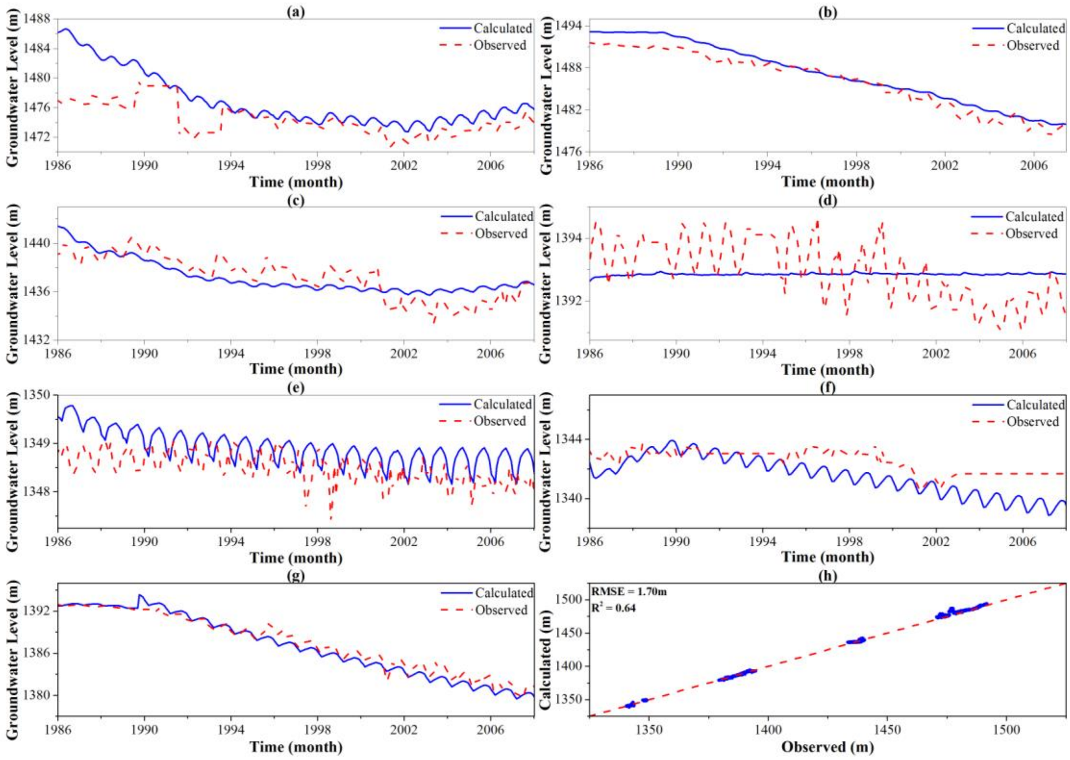

Fig. 7. Comparison between observed and simulated groundwater levels ((a) Daman; (b) ZhangYNC; (c) 54; (d) BanQDW; (e) 32; (f) SanYiQv; (g) 11)

4.2 Groundwater level assimilation and parameter estimation

In general, the groundwater system is simulated and analyzed by numerical models. However, numerical models would be inapplicable in a situation where aquifer parameters vary with time. Therefore, a recursive strategy was applied to capture the time variation of the hydraulic conductivity during the assimilation period. A synthetic case was conducted to assimilate groundwater level, estimate parameters and analyze the uncertainty of the parameters simultaneously. The calculated groundwater level from the simulation (shown in Fig. 7) was used as observations to update the parameters. Similar to the simulation results, seven boreholes were selected to illustrate the assimilation results (Fig. 8). Horizontal hydraulic conductivities from 8 sub-zones were the parameters to be estimated and analyzed through PF (Fig. 9). One hundred particles for each of the parameters were randomly generated from a logarithmic normal distribution for the prior distribution of the parameters. The expectation and variance of the distribution for the parameters in each sub-zone were respectively set to the calibrated value (Table 1) and 0.3 according to [95]. SIR filtering in the parameter space was carried out at each time step. By implementing Bayesian statistical inference, the posterior distributions of the parameters were estimated. The mean value of the posterior distribution was supposed to be the optimal estimation for the current time step.

The uncertainties of the parameters were considered by random generating the parameters from a log-normal distribution. PF was used to reduce the parameter uncertainties by involving more observations which was reflected by the narrowing of the distributions of the parameters (Fig. 9). As the assimilation proceeded, the posterior mean estimates for all the parameters were converging. In the meantime, the calculated groundwater levels converged toward the observations which indicated the reduction of the parameters uncertainties. The processes of reducing uncertainty in sub-zone 2 and sub-zone 5 were slower than in other sub-zones. This may be caused by the relatively less boreholes and centralized distribution of boreholes. Moreover, the interactions and transformations between groundwater and the Heihe River, the interactions between groundwater and boundary were both significant in this area. In other words, the information obtained from observations of sub-zone 2 and sub-zone 5 was not sufficient to reduce the uncertainties in these two sub-zones. Another reason for the different convergence rates was the small difference between the variance of the log-normal distribution for resampling and the relatively large value of the parameters. This would lead to small difference between the weights of different particles and less updating effects. Significant reductions of uncertainties for the other six parameters were observed after about 120 assimilation steps (around 1996). All the parameters were converged after about 144 assimilation steps (around 1998). The reason for these significant reduction could be attributed to the key role of new observation data (observed groundwater levels) in updating (correcting) of parameters. Because of the lack of observation wells in sub-zone 2 and sub-zone 7, the uncertainties remained large until the end of the assimilation period.

Furthermore, EnKF [18] was used to assimilate observations for the purpose of comparison with PF. In this experiment, the observations, parameters and numerical model were identical with regards to that in the PF case study. The results from PF and EnKF were shown in Fig. 10. A quantitative comparison of the results in all the boreholes was carried out to evaluate the performances of different algorithms. Generally, the differences between PF and EnKF were negligible. However, the results from PF were slightly better than those from EnKF. This may be caused by the nonlinearity and non-Gaussian distribution of the numerical model.

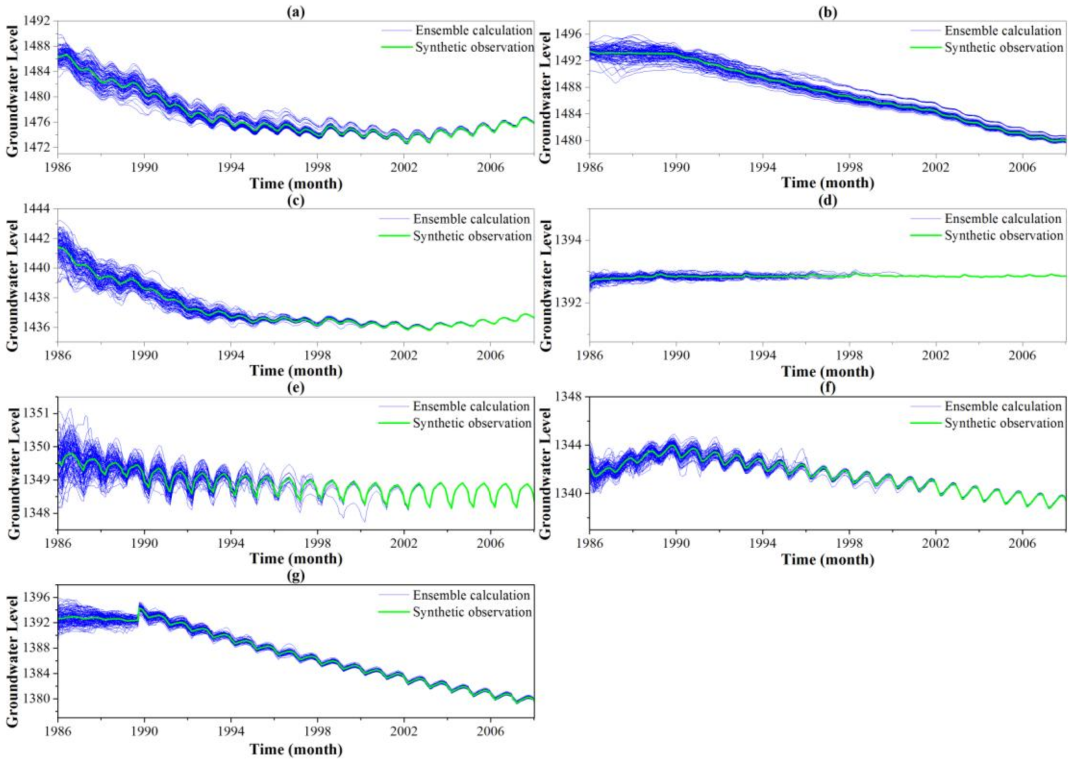

Fig. 8. The evolutions of groundwater level at observation wells ((a) Daman; (b) ZhangYNC; (c) 54; (d) BanQDW; (e) 32; (f) SanYiQv; (g) 11)

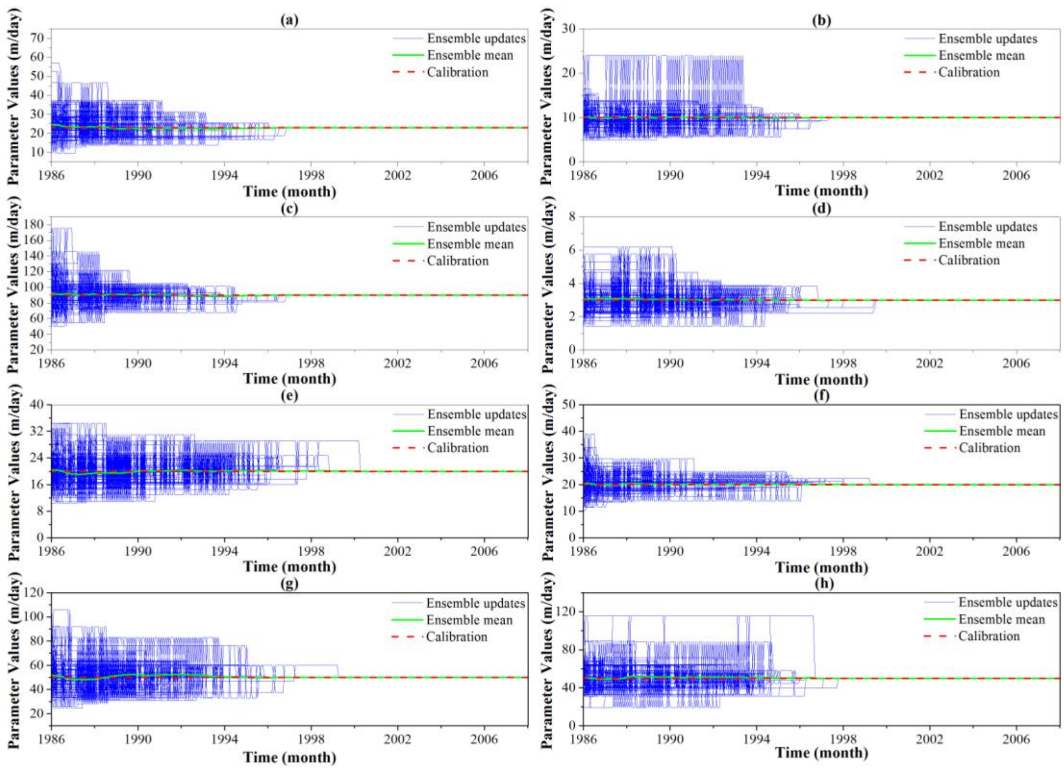

Fig. 9. The evolutions of hydraulic conductivities for sub-zones ((a) sub-zone 1; (b) sub-zone 2; (C) sub-zone 3; (d) sub-zone 4; (e) sub-zone 5; (f) sub-zone 6; (g) sub-zone 7; (h) sub-zone 8)

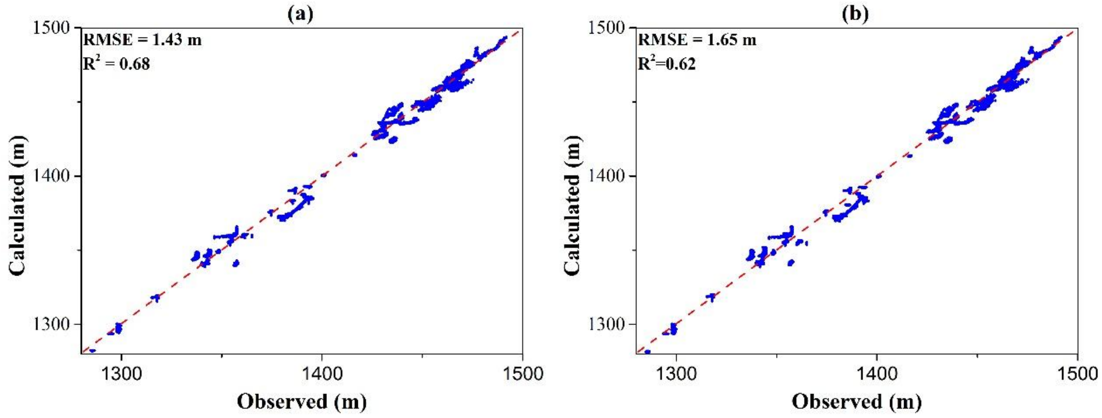

Fig. 10. Comparison of the results from PF and EnKF ((a) PF; (b) EnKF)

4.3 Groundwater model as a service

With the advancement of Information and Communications Technology (ICT), cloud computing emerges as one of the most inspiring technologies and widely used in many fields due to its cost efficiency and flexibility [96]. There is a trend that the computing resources are provided as services which results in IaaS, PaaS, SaaS and DaaS, etc. The groundwater model established in this paper was implemented on cloud to offer services for the users (decision makers, researchers, water managers, etc.).

In the RaaS architecture which was proposed by [36, 37], hardware components (e.g., intelligent things and robot) were connected to the cloud environment and provided to the RaaS users as a service. Similar to the RaaS, in MaaS architecture, the numerical model was implemented in the cloud environment and provided as services which were used to simulate different physical processes (irrigation, precipitation, evapotranspiration, groundwater pumping, river seepage, etc.) (shown in Fig. 11). Generally, a physical process was encapsulated as a service. Different services were able to cooperate with each other. The users were able to customize the services and formulate their own models for special problems. The establishment of the numerical model was not needed for the users which avoided the duplication of work. Furthermore, different models (e.g., groundwater models and crop growth dynamic models) were able to be integrated to consider the interactions and feedbacks between different processes. The visualization of observations and influence of different parameters and processes facilitated the decision-making processes for the MaaS users.

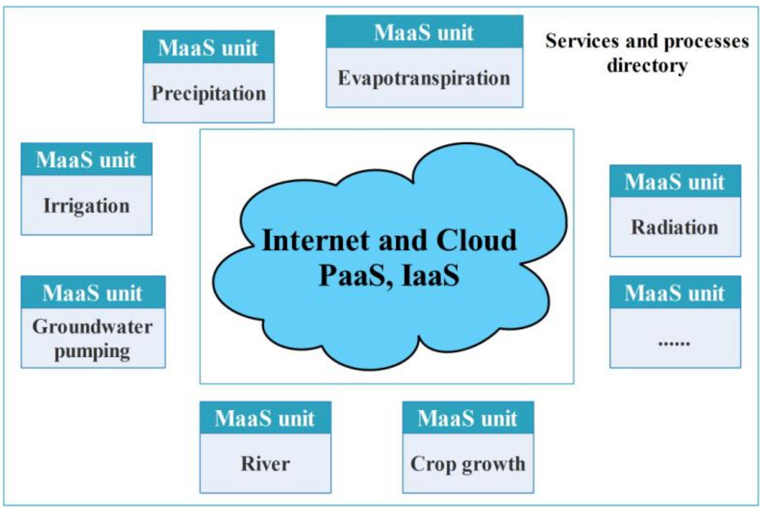

Fig. 11. MaaS in cloud environment.

4.4 Implementation of MaaS

To prove the concept of MaaS, we implemented the established groundwater model in the cloud environment as a case study. Fig. 12 showed the system consisting of the cloud (left) and the groundwater model which simulated several physical processes (i.e., Irrigation, Groundwater pumping, River and Evapotranspiration). The data and model settings of MaaS were presented previously. The deployment of the cloud environment engaged two general Personal Computers. On the software side, standard interface, Web capacity and distributed deployment were the main consideration.

- **Operating system:** The system was implemented on two Ubuntu-based machines.
- **Programming language:** NODE.JS was used to program the groundwater model into Web services.
- **Database:** MongoDB—a distributed document-oriented database—was deployed in the two Ubuntu-based machines to store the observations and the simulated data from the groundwater model.

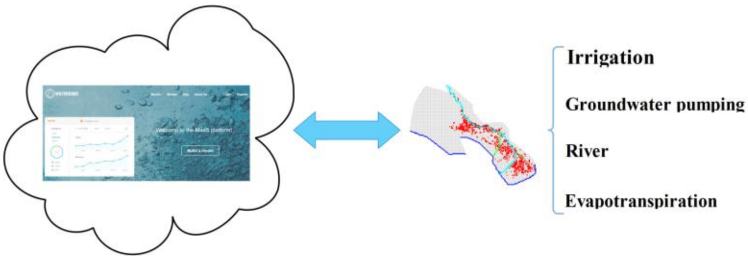

Fig. 12. MaaS in cloud environment (using groundwater model as a case study).

As shown in Fig. 13, some interfaces for basic features were provided as a service in the initial version. In the main page, the MaaS users were able to choose the layers (study area boundary, irrigation channels and observation wells) to load. The simulation period was limited from January 1986 to December 2008 and could be customized. The hydraulic conductivities for each sub-zone of the study area could be changed by the users for different purpose. Default parameter values were pre-defined by the calibrated values. After finishing the settings, the groundwater model was able to execute on the cloud. There was no need for the users to install or construct the model. The construction, data pre-process, model calibration, output post-process and visualization procedures were all handled by the system. The visualization for results was shown in Fig. 14. The observation boreholes were represented by the red marks in the study area. The observed groundwater level was available at each observation boreholes as shown in Fig. 14. By clicking the red marks, the time series of observed and calculated groundwater level were plotted. In the meantime, the calculated spatial distribution of the groundwater level was plotted in the form of heat map in the study area. Additional map layers were available to verify the reasonableness of the simulation results. The MaaS users can analyze the trend of groundwater level or the effects of different parameters or inputs on the groundwater system.

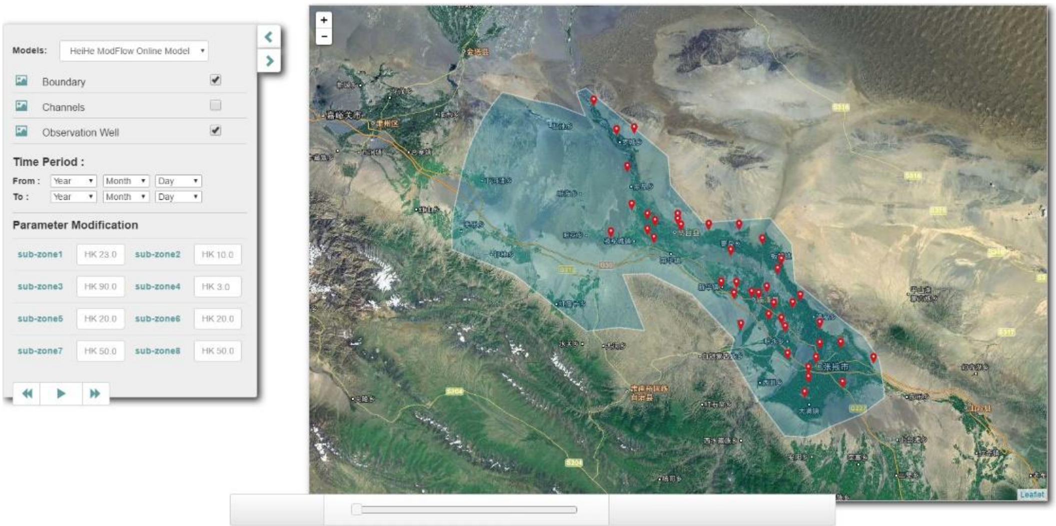

Fig. 13. Main page for MaaS

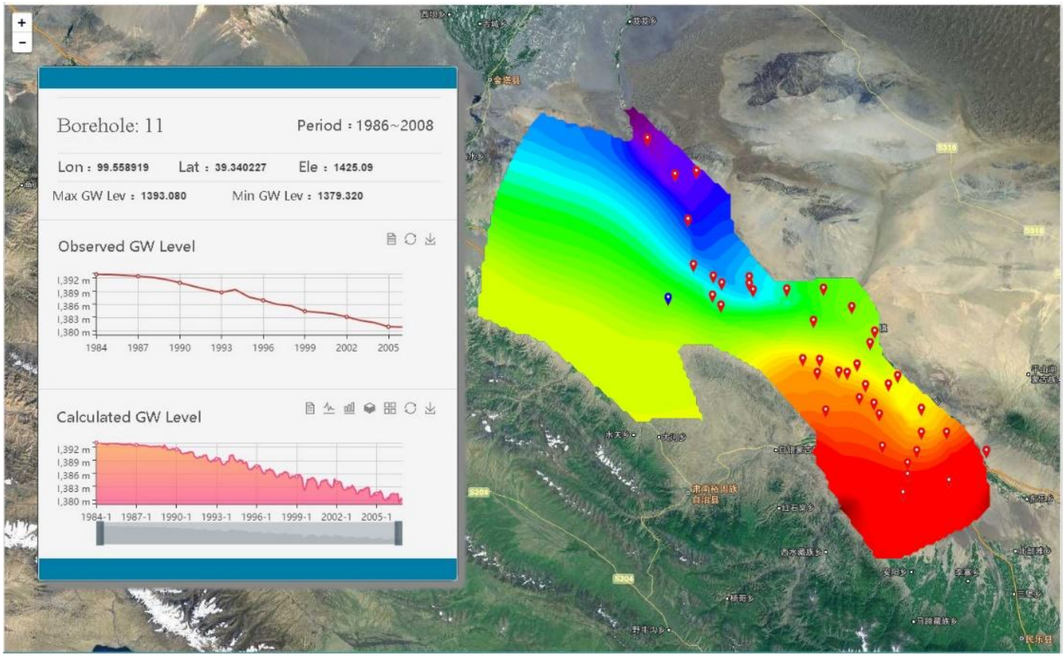

Fig. 14. Results from MaaS

5. Conclusions

As cloud computing becoming more and more popular, a new architecture of cloud computing—Model as a Service (MaaS) was proposed in this paper. A groundwater model of the middle reaches of the HRB in northwestern China was established to illustrate the advantages of MaaS. The groundwater model was adequately calibrated with observed groundwater level. The calibrated model reproduced the historical observations considerably at the monthly time scales. A sequential data assimilation method (Particle Filter) was developed to assimilate the observed information into the groundwater model to estimate the aquifer parameters (horizontal hydraulic conductivity). By implementing PF, the uncertainties of the groundwater model parameters were reduced and the parameters were adjusted along with time. An initial implementation of MaaS was realized with which the users were able to conduct spatio-temporal analysis of the observed and calculated groundwater level. The physical processes involved in the numerical model were realized as services on the cloud. The MaaS users were able to build their own models based on different services instead of establishing numerical models from scratch. However, the assumption that the aquifers were characterized only by hydraulic conductivities should be extended and more features for the MaaS should be provided in the future work.

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