Geosci. Model Dev. Discuss., 6, 4511–4530, 2013
www.geosci-model-dev-discuss.net/6/4511/2013/
doi:10.5194/gmdd-6-4511-2013

Geoscientific Model Development Discussions
Open Access

On searching for optimized set of physical parameterization schemes in a multi-physics land surface process model

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Received: 15 July 2013 – Accepted: 16 August 2013 – Published: 5 September 2013

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Published by Copernicus Publications on behalf of the European Geosciences Union.

Abstract

Optimization of land surface models has been very challenging due to the increasing complexity of such models. Typical parameter calibration techniques often limit the solution of the spatiotemporal discrepancy in the modeling performance levels especially for regional applications. Thus, in this study, an attempt was made to perform scheme-based model optimization by designing a framework for coupling a micro-genetic algorithm (micro-GA) with the Noah land surface model that has multiple physics options (Noah-MP). Micro-GA controls the scheme selections in 10 different land surface parameterization fields in Noah-MP in order to extract the optimal scheme combination for a certain region. This coupling framework was successfully applied to the optimization of the surface water partitioning in the Korean Peninsula, promising not only the effectiveness of the scheme-based optimization but also model diagnosis capability by exploring the scheme sensitivity during the micro-GA evolution process. Then, the method was applied to four different regions in East Asia that have different climatic characteristics. The results indicate that (1) the optimal scheme combinations vary with the regions, (2) schemes related to the surface water partitioning are important for the modeling accuracy, and (3) specialized post-parameter optimization for each region may be required.

1 Introduction

Land surface models (LSMs) have been significantly advanced in recent years, but their optimization has been increasingly challenging due to their increasing complexities and number of uncertainties, which require tremendous computing resources. LSMs are generally developed to represent better regional characteristics of surface hydrology, biophysics, and bio-geochemistry characteristics in terms of the interactions between land and atmosphere. However, models inevitably have uncertainties due to the insufficient knowledge of the nature. The uncertainties often arise from the unreasonable representation of the spatiotemporal surface heterogeneity. In order to resolve this issue for more extensive application studies, model optimizations through parameter calibrations have been essentially used. The widely used methods that apply model runs to regional scale studies include model optimizations by calibrating uncertain parameters based on observations. Such methods include parameter sensitive analyses for effective optimizations (Gupta et al., 2000; Jackson et al., 2003; Mo et al., 2008; Nasonova et al., 2011; Rosero et al., 2010; Williams and Maxwell, 2011). To make model runs more reliable, some studies have calibrated several uncertain parameters in each scheme in a stepwise manner (Moriasi et al., 2007). However, this type of optimizations tends to be limited to only a few sites due to the tremendous computing resources and time.

Model optimization techniques that maximize the computation effectiveness were recently developed. One of the methods that are being increasingly used for model calibration is a genetic algorithm (GA). The fundamental concept of GA is the natural selections of genes (parameters) for object evolution as in Genetics (Holland, 1992). A marked advantage of GA is its smart search for an optimal combination of parameters by considering the interactions among various uncertain parameters. In light of this advantage, GA has been used for various numerical models and spotlighted as an effective and reliable technique for handling the issues of the quantitative increase in uncertain parameters and the difficulty of regional applications of numerical models (Fang et al., 2003; Yu et al., 2013).

Another considerable problem in model optimizations is its possible conflicts with the already implemented schemes in a complex model. For example, significant improvement of a single physical process through certain parameter optimizations can be followed by exacerbations of other processes. However, this conflict may not be sufficiently addressed by considering merely uncertain parameter interactions, because the increasing complexity of models is not only associated with the increases in the number of uncertain parameters but also with augmentations of new parameterizing schemes. Rosero et al. (2010) revealed that the model sensitivitiy to parameters can vary according to the choice of scheme as well as parameters associated with land surface heterogeneity. Their study implies that interactions among the implemented schemes in a model may induce further considerable uncertainty for model optimization. This issue is very important when constructing a new model from various pre-developed parameterization schemes for their regional applications.

In the preceding context, it was asked if an optimized land surface mode can be created only by considering the scheme interactions via a GA and then if such methodology can be worthy for regional applications such as minimization of the spatial discrepancy in simulation performances. We used an efficient version of GAs, so-called micro-GA, that uses a small number of investigation samples. For this experiment, a framework for coupling micro-GA with a multi-physics LSM was designed, the effectiveness and reliability of the micro-GA applications were tested to extract the best scheme combination, and then this methodology was applied to several different regions in East Asia.

2 Methods

2.1 Noah LSM with multiple physics options

For a multi-scheme-available LSM, a new version of the Noah LSM with multiple physics options (hereinafter Noah-MP) was used. The Noah LSM has been evolved through the cooperative efforts of various institutions such as the National Center for Environmental Prediction and the Air Force Weather Agency. Using Noah LSM 3.0v as the baseline, Noah-MP was augmented with multiple physics options with regard to 10 different land surface processes (Niu et al., 2011). The augmentations were basically intended to improve the Noah LSM such as with respect to its inability to compute phenology, its simplified snow treatment, and its unrealistic groundwater representation. Among the ten physical fields, dynamic vegetation and its paired scheme for the stomatal resistance, the Ball-Berry scheme (Ball et al., 1987; Collatz et al., 1991), were

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fixed. Thus, eight parameterizing fields were totally used to generate scheme combinations as summarized in Table 1. The detailed descriptions of each scheme including equations and parameter settings can be found in the study of Niu et al. (2011).

2.2 Micro-GA

GAs, the idea behind which was borrowed from biological evolution and adaptation concepts in genetics, are heuristic optimization methods based on natural genetic variation and natural selection that pursue a cost-effective solution (Holland, 1992; Mitchell, 1998; Wang et al., 2002; Hu et al., 2006). These methods have been increasingly applied to parameter optimizations in various hydrological models (Bastani et al., 2010; Bulatewicz et al., 2009; Lee et al., 2006; Uddameri and Kuchanur, 2007) and to those in numerical weather predictions (Fang et al., 2009; Krishnakumar, 1989). Their fundamental mechanism in model optimization is to evaluate individuals in a group (or generation) to select an elite based on a fitness function and then to reproduce the next improved generation through stochastic modifications such as crossover and mutation of the elite in the previous generation. While the reproductions are repeated, the generations evolve and converge to the optimum. Micro-GA is an improved version of GA with smaller generation sizes and simplified genetic modifications, hence efficiently reducing the computational resources (Krishnakumar, 1989; Wang et al., 2010; Reeves, 1993).

2.2.1 Coupling micro-GA with Noah-MP

Micro-GA was applied for the scheme-based optimization using Noah-MP (hereinafter MP-MGA). The generation of a combination of schemes from various multi-optional physical processes is easily controlled with discrete numbers using micro-GA. In the MP-MGA, micro-GA controls the choices of physical schemes to produce scheme-generations and conducts a series of model runs using Noah-MP. The flow chart in Fig. 1 summarizes the optimization process in MP-MGA. Two basic parameters must

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be set to operate micro-GA: the number of individuals in a generation and the number of generations. Each generation was set at 10 individuals (scheme combinations) and the number of generations was set through the validation experiment (see Sect. 3). Once the micro-GA produces a random initial scheme combination, it runs Noah-MP and collects the skill scores for a generation based on the fitness function. From the skill scores for all the individuals, micro-GA selects the individuals with the best skill scores (Elitism) and reproduces the next generation by interchanging the scheme selections of the surviving individuals in order to induce evolution of the generations. This process above is iterated until the evolutions of the generations are converged enough to the global maximum that is the true optimum state.

2.2.2 Fitness function

Evaluation skills used in the fitness function are very subjective, depending on the study objectives. In this study, one of the common statistical indices, the Nash–Sutcliffe efficiency (NSE) (Nash and Sutcliffe, 1970), which is widely used in the hydrological modeling fields, was selected. NSE is a statistical index that evaluates the predictability of a model with respect to a certain variable, comparing the model's outputs to a reference data. However, since micro-GA uses only one evaluating fitness function, a special strategy is required to perform multi-variable evaluations. Thus, targeting two basic surface water components, evapotranspiration (ET) and runoff, a simple addition of the two individual NSEs was used as follows (mNSE).

$$\mathrm{mNSE} = \left\{ 1 - \frac{\sum_{i=1}^{n} \left(R_{\mathrm{ET},i} - V_{\mathrm{ET},i} \right)^2}{\sum_{i=1}^{n} \left(R_{\mathrm{ET},i} - R_{\mathrm{ET,mean}} \right)^2} \right\} + \left\{ 1 - \frac{\sum_{i=1}^{n} \left(R_{\mathrm{Runoff},i} - V_{\mathrm{Runoff},i} \right)^2}{\sum_{i=1}^{n} \left(R_{\mathrm{Runoff},i} - R_{\mathrm{Runoff,mean}} \right)^2} \right\} \tag{1}$$

where R refers to the reference data and V is the model output. Thus, mNSE ranges from 2 (perfect agreement) to negative infinity.

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2.3 Study domain and data

The land surface processes in the model were forced by six meteorological fields from the Global Land Data Assimilation System (GLDAS) data (Rodell et al., 2004): (1) precipitation, (2) downward shortwave radiation, (3) downward longwave radiation, (4) near-surface air temperature, (5) near-surface wind speed, and (6) surface pressure. The 10 yr GLDAS forcing data from 2001 was processed for four different regions in East Asia as the model forcing input. The previous six month data (July to December 2000) were utilized for the model initialization. As shown in Fig. 2, the four regions that have very different climatic characteristics were selected based on precipitation regimes for the regional applications of MP-MGA: (1) KOR (Korean Peninsula), (2) RE1 (the East Siberia), (3) RE2 (Gobi Desert), and (4) RE3 (South China). The different climates in the four regions are as follows: semi-humid (KOR), semi-arid (RE1), arid (RE2), and humid (RE3). An MP-MGA evaluation of KOR was performed for a shorter (three-year) simulation period (see Sect. 3). Then, MP-MGA was applied to all the study regions with a simulation period of 10 yr to investigate the differences in the optimal scheme combinations under different climatic patterns.

For the multi-variable evaluations, ERA-Interim was used for the reference data (Dee et al., 2011). ERA-Interim produced by the European Centre for Medium-range Weather Forecasts (ECMWF) is a global atmospheric reanalysis describing the states of the atmosphere, land, and ocean waves, which employed the four-dimensional variational assimilation. As the land surface component, ERA-Interim used the Tiled ECMWF Surface Scheme for Exchange over Land (Van den Hurk et al., 2000; Viterbo and Beljaars, 1995; Viterbo et al., 1999).

The models were evaluated through daily-averaged comparisons after the area aggregations were completed for the four regions in East Asia. The actual spatial and temporal resolutions in the simulations were 0.25 degrees and 3 h, respectively. The first 6-month outputs were excluded as the period for the model initialization.

3 Evaluation of MP_MGA for the scheme-based optimization

This section addresses the evaluation of MP-MGA, in terms of capability and efficiency by comparing 3 yr simulations in the Noah-MP stand-alone mode and the MP-MGA coupled mode. The best skill score (or mNSE) that was obtained from the all the 1728 simulations for KOR was 0.62. Then experiments with MP-MGA were performed to examine how fast MP-MGA reaches the global maximum (the best skill score). Figure 3 shows the evolution of generations with the increase in the number of generations, each of which is composed of 10 individuals (i.e. scheme combinations). MP-MGA reached the maximized evolution at the 10th generation and found the global maximum at the 9th generation. This indicates that only about 100 simulations are enough to obtain the optimal MP-MGA output. The fast decrease in the average skill score right after the 10th generation indicates the restarting point at which the evolved generation is reset with random selection plus the best individual from the previous iteration when the percentage of the number of different bits between the best individual and other members in a generation is less than 5 %. This process is important to reduce the possibility of convergence into any local maximum (or false optimization). The maximum evolution was restored at the 15th generation.

Another interesting capability of MP-MGA is that it can provision of the information on model sensitivity to scheme choices in terms of the model accuracy (more precisely, the simulation accuracy of the selected variables) through the evolution process of the generations. For example, the MP-MGA log revealed that the sudden degeneration at the 11th generation was due to the choices of the runoff scheme field (RUN). This indicates that the main contributor to the improvement of the model accuracy is the choices in RUN. This sensitivity analysis to scheme selections can be performed more easily but more clearly by simply counting the schemes selected via MP-MGA. Through the natural selection mechanism, micro-GA essentially selects a greater number of better individuals for evolution. Therefore, the greater number of selections of a certain scheme through the process accounts for its higher contribution to the model accuracy.

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For example, according to the log, RUN (1) is exclusively presented in 30 % of the top-ranked of all MP-MGA selections. ALB (2), the second contributor, also shows a very high portion (about 80 %) of 30 % of the top-ranked ones. These results are consistent with those of the analyses of all Noah-MP simulations and indicate the capability of MP-MGA to be a tool for scheme sensitivity tests.

4 Applications of MP-MGA in East Asia

Full 10 yr simulations using MP-MGA with 15 generations were performed for the four study regions in East Asia. Thus, 150 simulations in all were performed for each region. Figure 4 shows the final (the best and worst) MP-MGA outputs. Table 2 summarizes the selected schemes that were selected for their best simulation performances for each region from the MP-MGA extractions. The results show that the scheme combinations varied with the region, possibly in association with the regional climate.

Among the four regions, the best scheme combinations were extracted from MP-MGA for KOR and RE1, which have moderate climate conditions. They showed relatively reasonable performances in the runoff and ET. Among the schemes that were chosen for KOR, the schemes that mainly contributed to the accuracy achievement were RUN (1), ALB (2), and SFC (1) The results were similar to those obtained from the 3 yr MP-MGA coupling test that was mentioned in Sect. 3. As shown in Fig. 4, the best extracted runoff outputs were consistent with the reference data, and the best extracted ET outputs showed reasonable quantitative acquisition in the summer but underestimation in winter. To improve the model estimation of the winter ET for this region, parameter optimizations within the extracted schemes may be required, especially for those involved with winter variations (e.g. the ALB schemes). RE1 shows good performances in ET simulation but some underestimation of the runoff. In this region, compared to KOR, the overall model performance was strongly affected by the ET simulation. The schemes that contributes most to the achievement of the best mNSE over RE1 were SFC (1) and INF (1), which are considered to be mainly involved in the ET simulations. From the comparisons of the best and worst runoff simulations, it is inferred that the choices of schemes and/or their combinations affect not only the systematic errors but also the temporal variations.

On the other hand, RE2 and RE3 showed relatively poor simulation performances. No scheme choices or their combinations for ET over RE2 had better impact on the model performance. However, the MP-MGA exploration (i.e. in the arid region) was good at least for reasonable acquisition of surface water partition, e.g. by reducing the runoff estimation. While RE3 performed relatively well in the runoff simulation, its ET results were very poor, showing very different seasonal variations. The schemes related to the ET estimation may need to be improved with further parameter optimization for reasonable ET seasonality.

It is notable that the selection of the scheme in SFC was important in all the regions except in RE2. In SFC, the schemes define the characteristics of heat exchange between land and atmosphere, and thus play an important role in determining the proper partitioning of surface water, thereby affecting the simulation accuracy of ET and runoff.

5 Summary and conclusions

This study was conducted to design a framework for scheme-based model optimization by coupling an intelligent model optimization technique to the multi-physics land surface model. Micro-GA, which enables smart searching for the optimum case among numerous cases, was introduced and applied it to a new version of Noah LSM with multiple physics options. The experiment for the MP-MGA coupling over Korea Peninsular successfully demonstrated how micro-GA can effectively search the optimal physics combination from Noah-MP; only 150 of the 1728 simulations were needed to reach the global maximum. It should be noted that a proper setting of the number of itinerating generations in micro-GA is essentially important to avoid being trapped into any local maximum. Additionally, this study shows a potential applicability of the coupling method to model diagnosis. That is, the natural selection mechanism through the micro-GA's evolutionary process of generations provides information on scheme sensitivity and interrelationships. Then, this method was applied to four different areas in East Asia. These experiments provided information on which scheme contributes more to simulation accuracy for regions with different characteristics. Such information will be useful for further improvement for better accuracy through either parameter optimizations or scheme developments with the consideration of various regional characteristics. In addition, as the optimized scheme combinations vary with regions, a numerical model might need to have multiple scheme-combinations, each of which is specifically optimized for a certain region in order to minimize the spatiotemporal discrepancy of model's simulating performances.

Overall, the interface of a micro-GA to Noah-MP was successfully implemented, and the coupled MP-MGA system turned out to be very useful in identifying an optimized set of physical schemes for Noah-MP. The framework that was designed in this study is expected to have high applicability for model developments. It promises effective management of uncertainties in any inevitable circumstance (e.g. the increases in the model's uncertainties). This kind of system can be a useful tool for comprehensive evaluation of a newly augmented scheme that has interrelationships with various implemented schemes. This may also enable specialized model calibrations for models' representations of existing diversities in regional characteristics such as in their climate, hydrology, geography, and so on.

Acknowledgements. The authors are grateful to the anonymous reviewers for their constructive comments. Thanks are also given to the Goddard Earth Sciences (GES) Data and Information Services Center (DISC) and ECMWF for providing the GLDAS and ERA-Interim data, respectively. This work was supported by the National Research Foundation of Korea (NRF) grant funded by the Korea government (MSIP) (No. 2009-83527).

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Table 1. Summary of scheme options available in Noah-MP.

Parameterizing fields	Available schemes
Soil Moisture Factor controlling stomatal resistance, β factor (SMF)	(1) Noah type; (2) CLM type; (3) SSiB type
Runoff and Groundwater (RUN)	(1) SIMGM; (2) SIMTOP; (3) Free-drainage scheme; (4) BATS
Surface exchange coefficient for heat, CH (SFC)	(1) Noah type; (2) Monin-Obukhov scheme
Supercooled liquid water in frozen soil (FRZ)	(1) Generalized freezing-point depression; (2) Variant freezing-point depression
Frozen soil permeability (INF)	(1) Defined by soil moisture; (2) Defined by liquid water volume
Two-stream radiation transfer (RAD)	(1) Canopy gaps from 3-D structure and solar zenith angle; (2) No canopy gap; (3) Gaps from vegetated fraction
Snow surface albedo (ALB)	(1) BATS; (2) CLASS
Partitioning precipitation into rain and snow (PRT)	(1) Complex functional form; (2) Snowfall at $T_{air} < T_{frz} + 2.2$ K; (3) Snowfall at $T_{air} < T_{frz}$

CLM (Community Land Model); SsiB (Simple Simplified Biosphere Model); SIMGM (Simple Groundwater Model); SIMTOP (Simple TOP Runoff Model); BATS (Biosphere-Atmosphere Transfer Model); CLASS (Canadian Land Surface Scheme).

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Table 2. The best scheme combinations extracted from MP-MGA for each region. The italic-text schemes indicate the most contributing ones to the simulation accuracy based on mNSE.

Region	Scheme Combination	mNSE
KOR	*SFC(2)*; FRZ(2); INF(2); *ALB(2)*; *RUN(1)*; SMF(2); RAD(3); PRT(1)	0.64
RE1	*SFC(1)*; FRZ(2); *INF(1)*; ALB(2); RUN(2); SMF(1); RAD(2); PRT(3)	0.98
RE2	SFC(1); FRZ(2); *INF(2)*; ALB(2); RUN(4); *SMF(1)*; RAD(1); PRT(2)	−0.39
RE3	*SFC(2)*; FRZ(1); INF(2); ALB(1); *RUN(1)*; *SMF(3)*; RAD(3); PRT(1)	0.07

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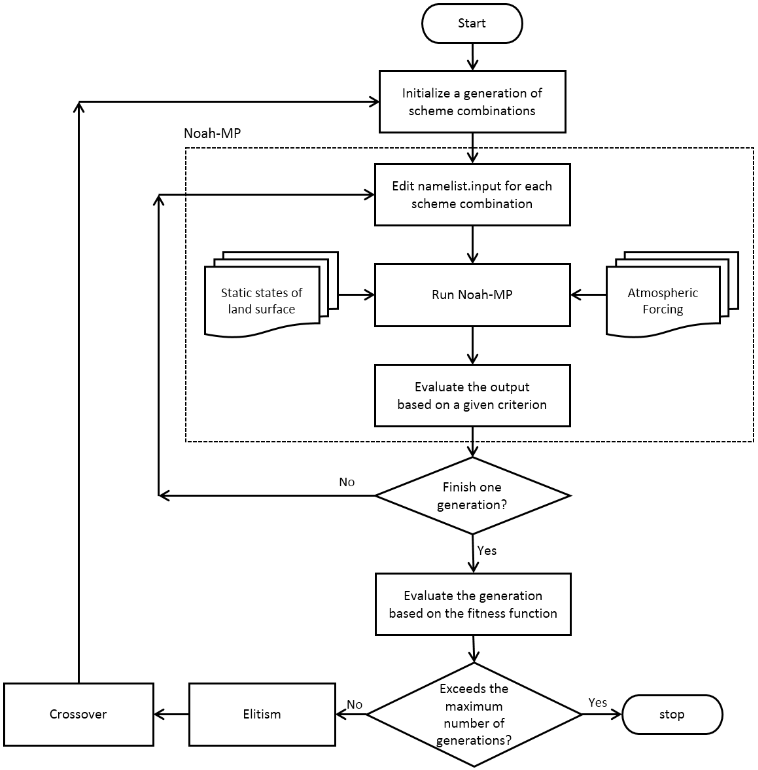

Fig. 1. A flow chart describing the scheme-based optimization process from the coupled micro-GA and Noah-MP model.

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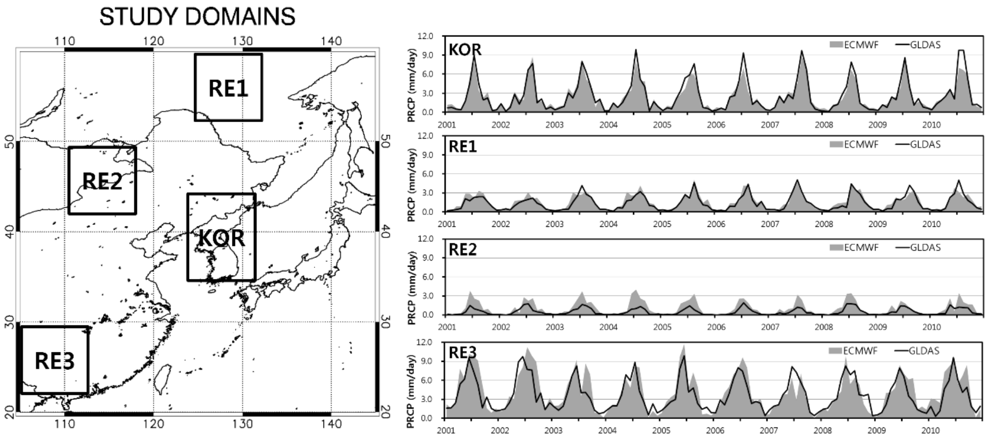

Fig. 2. Geographic locations of the four selected regions in East Asia and the precipitation regimes (plotted as 10 yr monthly mean variations).

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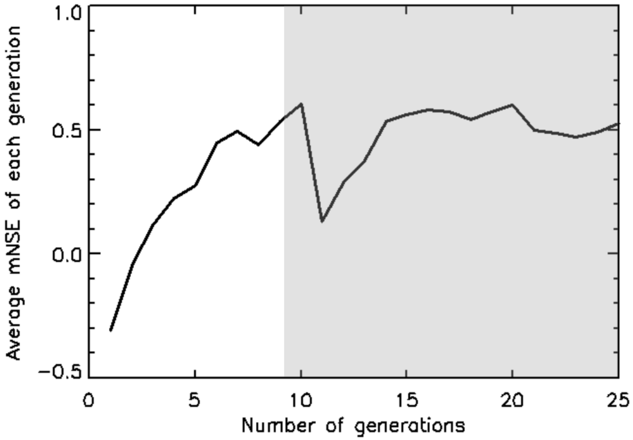

Fig. 3. Evolution of generations with the increase of iterations. The shaded area indicates the generations in which MP-MGA reached the global maximum.

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Optimized set of physical schemes in Noah-MP

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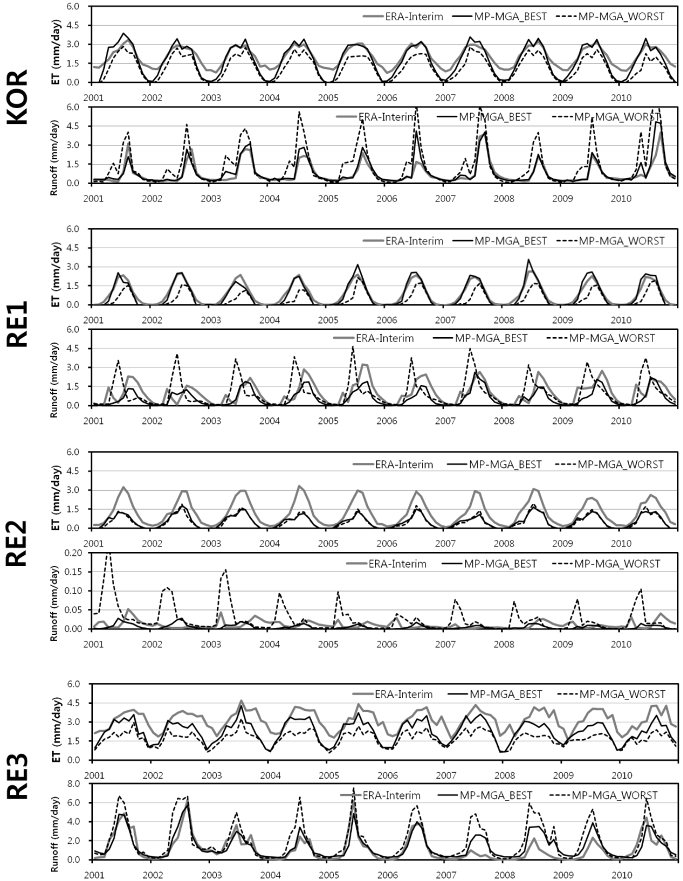

Fig. 4. 10 yr monthly variations of the best and worst outputs of ET and runoff from MP-MGA (solid and dashed lines, respectively) and ERA-Interim (thick gray lines) for each region.