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Coupling Simulation and Optimization to Solve Planning Problems in a Fast-Developing Area

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In geographical analysis, spatial simulation and optimization are usually separate processes tackling different problems. It is, however, increasingly necessary to integrate them. Particularly in a fast developing area, the development to be simulated is seldom inertial (i.e., strictly following the historical trend); instead, it is likely to be interfered by new planning measures. Meanwhile, in such an area an optimization plan might not be even meaningful if it only addresses a snapshot of a highly dynamic landscape. In this study, we explored the possibility of integrating cellular automata (CA), a widely used method for simulating urban development and land use changes, and ant colony optimization (ACO), an advanced technique for solving complex path optimization problems. We named the resulting integrated system the geographical simulation and optimization system (GeoSOS) and applied it to a case study concerning finding the optimal path for a planned expressway in Dongguan, a fast-growing city in one of the most economically active regions of China. In the case study, the CA component of the GeoSOS generated simulations of the industrial land use changes for some years in the next decade. The ACO component of the GeoSOS, which had been revised from the conventional ACO to work on raster surfaces, took the simulations as input and completed raster-based path optimizations. In terms of the cumulative utility, a measurement used to evaluate the performance of the optimization, the coupling method surpasses the noncoupling method by 10.3 percent. Key Words: ant colony optimization, cellular automata, land use simulation, model coupling, path optimization.

在地理分析中,空间模拟和优化通常是应付不同的问题的分开的过程。但是,集成他们是越来越必要的。尤其是在快速 发展地区,被模拟的发展是很少惯性的(即严格追随历史趋势),相反,它很可能是被新的规划措施干扰。同时,在这样 一个地区的一个优化方案,甚至可能没有意义,如果它只处理了高度动态景观的一个快照。在这项研究中,我们探讨了 整合细胞自动机(CA),一个模拟城市发展和上地利用变化的广泛使用的方法,和蚁群算法(ACO),一个为解决复杂的 路径优化问题的先进技术,的可能性。我们把产生的综合系统命名为地理模拟优化系统(GeoSOS),并将其应用到东 莞,中国经济最活跃的地区之一的一个快速发展的城市,为其一条规划的高速公路寻找最佳路径的案例研究,在此案例 研究中,该 GeoSOS的CA组件生成了未来十年中的一些年工业用地变化的模拟。该 GeoSOS的ACO组件,已经从传 统的ACO修订到栅格表面的工作,把模拟作为输入并完成了基于栅格的路径优化。在累积效用上,即一个用于评估优化 性能的测量,耦合方法优于非耦合方法 10.3%。关键词:蚁群优化算法,元胞自动机,土地使用模拟,模型耦合,路径 优化。

En análisis geográfico la simulación y optimización espaciales usualmente son procesos separados que abordan problemas diferentes. Sin embargo, cada vez se hace más necesario integrarlos. En particular en una región que se desarrolle con rapidez, el desarrollo que se deba simular rara vez sigue la inercia (o sea, que siga estrictamente la tendencia histórica); en vez de eso, lo más seguro es que sea interferido por nuevas medidas de planificación. Mientras tanto, en tal tipo de área un plan de optimización podría no ser siquiera significativo si apenas cubriera una fracción de un paisaje altamente dinámico. En este estudio exploramos la posibilidad de integrar autómata celular (AC), un método ampliamente utilizado para simular desarrollo urbano y cambios en el uso del suelo, y optimización de hormiguero (ACO), una técnica avanzada para solucionar problemas de optimización de ruta compleja. Al sistema integrado que resultó lo denominamos sistema geográfico de simulación y optimización (GeoSOS), el cual aplicamos a un estudio de caso dedicado a encontrar la ruta óptima para una supercarretera planificada en Dongguan, una ciudad de rápido crecimiento en una de las regiones económicamente más activas de China. En el estudio del caso, el componente CA del GeoSOS generó simulaciones de los cambios en uso del suelo industrial para algunos años de la próxima década. El componente ACO del GeoSOS, que había sido revisado del ACO convencional para trabajar en superficies *raster*, tomó las simulaciones como insumos y completó las optimizaciones de ruta de base *raster*. En términos de la utilidad acumulativa, medida usada para

evaluar el desempeño de la optimización, el método de acoplamiento sobrepasa al método sin acople en un 10.3 por ciento. Palabras clave: optimización de hormiguero, autómata celular, simulación del uso del suelo, modelo de acoplamiento, optimización de ruta.

There is a rich literature on geo-simulation and optimization for various geographical applications (e.g., Batty and Xie 1994; Clarke, Hoppen, and Gaydos 1997; Li and Yeh 2002, 2004; Bennett and Tang 2006; Manson 2006; Torrens 2006; Xiao, Bennett, and Armstrong 2007). In these applications, however, simulation and optimization are usually separate processes tackling different problems. To our knowledge, the integration of simulation and optimization in geographical applications is an area yet to be explored.

Simulation aims to generate realistic scenarios under given conditions, whereas the goal of optimization is to provide optimal solution(s) to a given planning problem. In terms of Yeh's framework that classifies the tasks of geographic information systems (GIS) in planning into three categories—description, prediction, and prescription (Yeh 1999)—simulation is a major approach to prediction, whereas optimization belongs to prescription. When being performed separately, simulation usually adopts an *inertial* strategy; that is, it assumes that future development will follow the historical trend (Liu et al. 2010), and optimization in most cases also assumes the problem to be static.

Increasingly, we see the need for coupling simulation and optimization in many geographical applications. Particularly in a fast developing area, on the one hand, the development to be simulated is seldom inertial; instead, it is likely to be interfered by new planning measures (which might or might not be optimal solutions). On the other hand, in such an area an optimization might not be even meaningful if it only addresses a snapshot of a highly dynamic landscape. As a result, for either simulation or optimization to be practically accurate and useful in this type of area, each needs to cooperate with the other. Specifically, if the primary concern is prediction, then the simulation should take into account the planning activities that are likely to occur or those the planners intend to evaluate and overlay such activities with the historical trend to generate realistic scenarios. If the primary concern is prescription, then the optimality of a solution should be evaluated based on a dynamic process rather than a snapshot, and the dynamics can be represented and characterized by a series of simulations. The former (the scenario that the primary concern is prediction) has been initially investigated by Li and Yeh (2002, 2004) and Liu et al. (2010). This study focuses on the latter scenario, in which the primary concern is prescription.

Previous studies have mainly focused on the development of separate simulation and optimization tools (Li and Yeh 2002, 2004; Li, He, and Liu 2009a, 2009b; Li et al. 2010). In this study, we explored a methodological approach of integrating simulation and optimization for solving an optimal path planning problem in a changing landscape. We have not found that this type of integration has been formally reported in the spatial analysis literature. The specific simulation method we brought to the integration is cellular automata (CA), a widely used method for simulating urban development and land use changes. The optimization method we tested is ant colony optimization (ACO), an advanced and relatively new technique for solving complex optimization problems. We named the resulting integrated system the geographical simulation and optimization system (GeoSOS) and applied it to a case study concerning finding the optimal path for a planned expressway in Dongguan, a fast-growing city in one of the most economically active regions of China.

The next two sections of this article describe the CA and ACO components of the GeoSOS, respectively, which is followed by a section detailing the integration of the two in the GeoSOS. The case study in Dongguan is then presented, followed by some conclusions drawn from this study.

Cellular Automata for Simulating Urban Land Use Changes

As a bottom-up approach, CA consists of a collection of discrete cells that represent spatial units, each in one of a finite number of states. The state of each cell evolves through a number of discrete time steps controlled by a set of transition rules. Basically, these rules define how a cell will evolve based on its own state and the states of its neighboring cells. This approach is attractive because it can represent, simulate, and reveal complex behaviors and patterns of geographical phenomena by using some simple rules (Batty and Xie 1994; Wu and Webster 1998). Simulation of complex urban systems is one of the successful applications of CA. Recent years have witnessed increasing study of the development of geographical CA for simulating urban expansion and land use dynamics (Batty and Xie 1994; Clarke, Hoppen, and Gaydos 1997; Li and Yeh 2002, 2004). Many such CA systems have generated encouraging results in solving various urban and regional simulation problems (Clarke, Hoppen, and Gaydos 1997; Wu and Webster 1998; Li and Yeh 2002, 2004; Wu 2002).

Generically, an urban CA model can be represented as follows:

$$S^{t+1} = f(S^t, N) \tag{1}$$

where S^t is the state of a cell at time point t, N represents a group of cells that are within the neighborhood of the cell under concern, and f is a transition function (i.e., rule) that governs the state transition from S^t to S^{t+1} .

In the past three decades, a major research topic in CA for urban simulation is how to define or derive transition rules. In most cases, transition rules are heuristically defined based on domain knowledge and expert's preferences. For example, the SLEUTH model (Clarke, Hoppen, and Gaydos 1997) that addresses four types of urban growth mechanisms, namely, spontaneous, new spreading center (diffusive), edge (organic), and road-influenced growth, is controlled by the factors of DIFFUSION, BREED, SPREAD, and SLOPE-**RESISTANCE**, and ROAD-GRAVITY. Other types of urban CA have been developed to capture these growth mechanisms by using the methods of multicriterion evaluation (MCE; Wu and Webster 1998), logistic regression (Wu 2002), neural networks (Li and Yeh 2002), decision trees (Li and Yeh 2004), and genetic algorithms (Li, Yang, and Liu 2008).

Among these different methods, logistic regression is relatively easy to implement and allows for the development probability to be straightforwardly derived through evaluating a suitability score that combines multiple factors. An early logistic regression CA was proposed by Wu (2002), which is an extension of MCE-CA (multicriterion evaluation CA) originally developed by Wu and Webster (1998). The basis of MCE is a suitability score obtained from a linear combination:

$$z_{ij}^{t} = a_{0} + a_{1}x_{1}^{t} + a_{2}x_{2}^{t} + \dots + a_{m}x_{m}^{t} + \dots + a_{M}x_{M}^{t}$$
(2)

where z_{ij}^t is the suitability score for urban development, a_0 is a constant, x_m^t is a spatial variable representing a

driving force for urban development at cell ij, and a_m is the weight of that variable.

This MCE method has difficulty using training data (e.g., land use maps or classified remote sensing data) to calibrate the CA. To facilitate the calibration, Wu (2002) transformed the method into a logistic form:

$$p_{ij}^{t} = \frac{\exp(z_{ij}^{t})}{1 + \exp(z_{ij}^{t})} = \frac{1}{1 + \exp(-z_{ij}^{t})}$$
(3)

where p_{ii}^t is the development probability at cell *ij*.

The preceding equation only addresses the global influences of the spatial factors. It ignores the fact that urban development is also subject to local influences (interactions) and that local interactions are the core of CA. In addition, no items in Equation 3 cover potential constraints and uncertainties, which are also critical factors in urban development. Therefore, Equation 3 should be further revised as follows (Wu 2002; Li, Yang, and Liu 2008):

$$p_{ij}^{t} = (1 + (-\ln\gamma)^{\alpha}) \frac{1}{1 + \exp(-z_{ij}^{t})}$$
$$\times f(\Omega_{ij}^{t}) \times con(s_{ij}^{t})$$
(4)

In Equation 4, γ is a stochastic factor ranging from 0 to 1 and α is a coefficient to control the stochastic degree. These two parameters represent the uncertainty in the urban development. $f(\Omega_{ij}^t)$ is a function characterizing the local interaction within the neighborhood of cell ii, and Li, Yang, and Liu (2008) implemented it as the count of all of the developed cells in the neighborhood of cell *ij*, which represents local development intensity. The function $con(s_{ij}^t)$ represents constraints that might apply to the development. In Li, Yang, and Liu (2008), this function was used to mask out all the unavailable sites for development, such as built-up areas, mountain areas, water bodies, and agricultural protection zones. At each iteration, p_{ii}^t is compared with a threshold *T* to determine if a nonurbanized cell will be converted into an urbanized cell:

$$S_{ij}^{t+1} = \begin{cases} Converted, & p_{ij}^t \ge T\\ NonConverted, & p_{ij}^t < T \end{cases}$$
(5)

The preceding logistic CA can be used to simulate urban development after the model has been calibrated by using two dates of land use maps or classified remote sensing data. The CA model proposed by Li, Yang, and Liu (2008) is the one we chose to use in this study.

Ant Colony Optimization for Path Finding

Researchers in spatial optimization have made efforts to develop models for facilitating multiobjective spatial decision making (Xiao, Bennett, and Armstrong 2007). A typical optimization task is site selection, with the objective of identifying optimal locations for siting a number of facilities, such as factories, schools, hospitals, shopping centers, and warehouses (Li and Yeh 2005). Another type of spatial optimization problem is related to linear features, particularly path finding, with applications in robot path planning (Kruusmaa and Willemson 2003), emergence evacuation, logistics management, infrastructure planning, and travel demand analysis (Tanga and Pun-Cheng 2004).

ACO, which was first proposed by Dorigo, Colorni, and Maniezzo (1991), is a method that tries to solve complex optimization problems according to simple searching behaviors of a large number of individuals (artificial ants). In this study, we chose ACO as the path optimization method to be coupled with the land use simulation.

A Brief Overview of ACO

ACO is a class of computer algorithms for solving combinatorial optimization problems. ACO was inspired by observations of the behaviors of ants in seeking food. In spite of the simplicity in the movement of each individual ant, an ant colony presents a highly structured social organization for completing complex tasks. By mimicking biological ants, researchers have shown that a group of cooperating artificial ants with simple intelligence can effectively solve complex optimization problems (Colorni, Dorigo, and Maniezzo 1991).

ACO is devised by simulating ants' behaviors of selecting the best route from a food source to their nest (Dorigo and Gambardella 1997). In ACO, artificial ants explore the environment to find a route and meanwhile lay down pheromones to direct each other. The positive feedback in the coordination among ants is achieved by exploiting the pheromones' communication mechanism. An early application of ACO was to solve the traveling salesman problem, which is to find a closed tour of minimal length connecting N given cities (Dorigo, Maniezzo, and Colorni 1996) over a road network. In the algorithm, an artificial ant's probability of going from its current city to another given city is determined by (1) the amount of pheromone on the path linking the two cities and (2) the visibility (measured by the travel distance between these two cities). In addition, a "taboo" list is used to prevent going back to a visited city. Formally, the probability for an ant to move from city u to city v is given as follows (Dorigo, Maniezzo, and Colorni 1996):

$$p_{uv}^{k}(t) = \begin{cases} \frac{\left[\tau_{uv}(t)\right]^{\alpha} \cdot \left[\eta_{uv}(t)\right]^{\beta}}{\sum\limits_{\substack{x \in S^{k} \\ 0}} \left[\tau_{ux}(t)\right]^{\alpha} \cdot \left[\eta_{ux}(t)\right]^{\beta}}, & \text{if } v \in S^{k} \\ 0 & \text{otherwise} \end{cases}$$
(6)

where p_{uv}^k is the probability of the *k*th ant to move from city *u* to city *v*; τ_{uv} is the amount of pheromone on path (u, v); η_{uv} is a heuristic function related to the visibility (distance); and S^k is the cities that the *k*th ant is allowed to visit. The *t* in the parentheses indicates that τ , η , and *p* are specific about time *t* (i.e., one iteration in the optimization). The parameters α and β control the relative importance of the pheromone versus the visibility (distance). A larger value of α means the probability is more influenced by the pheromone intensity, whereas a larger value of β allows the probability to rely more on the visibility (distance). At each iteration, the amount of pheromone on path (u, v) is updated as follows (Dorigo, Maniezzo, and Colorni 1996):

$$\tau_{uv}(t+1) = (1-\rho)\tau_{uv}(t) + \Delta\tau_{uv}(t) \tag{7}$$

where

$$\Delta \tau_{uv}(t) = \sum_{k=1}^{m} \Delta \tau_{uv}^{k}(t)$$
(8)

In Equation 7, ρ is a coefficient such that $(1 - \rho)$ represents the evaporation of the pheromone trail left by an ant between t and t+1; m is the total number of ants; and $\Delta \tau_{uv}^k(t)$ is a measurement of the intensity of pheromone left by the kth ant on path (u, v) between time t and t + 1, which is calculated as follows (Dorigo, Maniezzo, and Colorni 1996):

$$\Delta \tau_{uv}^{k}(t) = \begin{cases} \frac{Q}{L_{k}}, & \text{if the } k \text{th ant visits } (u, v) \\ 0, & \text{otherwise} \end{cases}$$
(9)

where Q is a constant, and L_k is the tour length or the total travel cost (from the origin to the destination) of the *k*th ant.

Equations 6 through 9 ensure that an ant will have a higher probability of selecting a shorter tour route (based on the explorations by all the ants in previous iterations). This is because (1) a shorter route has a higher intensity of pheromone left along it (Equation 9), and (2) there is a positive feedback between the number of ants that have chosen a path and the probability of another ant to choose the same path (Equation 7).

The heuristic function $\eta_{uv}(t)$ in Equation 6 is for reducing randomness in the path exploration and increasing the efficiency in converging to the desired route. It is defined as the inverse of the distance, d_{uv} , between cities u and v (Dorigo, Maniezzo, and Colorni 1996):

$$\eta_{uv}(t) = \frac{1}{d_{uv}} \tag{10}$$

Multiobjective Path Optimization over Raster Surface with ACO

The conventional ACO was developed to deal with a simplified scenario, in which the algorithm primarily considers only the cost along a vector network. A path optimization problem in regional or urban planning can be much more complicated. First, path optimization in planning usually involves multiple objectives that often conflict with one another. Typically, such an optimization intends to minimize the cost and maximize the coverage at the same time. Multiobjective path optimization can be difficult, because it might involve a huge solution space (Li and Yeh 2005). Second, most path-finding algorithms are based on vector networks (Jong, Jha, and Schonfeld 2000; Jong and Schonfeld 2003), as they require links (e.g., street lines) that connect different places and identify the optimal path by tracing adjacent nodes in a network (Current, Re Velle, and Cohon 1985). In regional or urban planning, however, sometimes optimal paths need to be generated from scratch; that is, they are not based on existing road networks or there is no existing road network at all (e.g., in a rural area), which makes a link-node-based algorithm difficult to implement. Another problem with the vector algorithms is that in real-world planning the cost and coverage of a path might not only be determined by the properties that can be attached to an entire link (e.g., the length of the link) but involve contextual properties that can vary continuously over space (e.g., slope gradient and distance to neighboring industrial facilities) and could be difficult to attach to discrete objects like links. Because of these problems, sometimes in regional or urban planning raster algorithms for path optimization are desired (Yu, Lee, and

Munro-Stasiuk 2003). Over a raster surface the path exploration is not based on and restricted by existing road networks, and representing continuously varying contextual information is relatively easy. Another advantage of raster-based path optimization is that it can directly take raster data provided by GIS and remote sensing as inputs and therefore is inherently compatible with the land use change simulation that is usually based on those raster data. Nevertheless, raster-based path optimization has its own difficulties that have seriously limited its uses in practice. A major problem of this type of algorithm is the slow (or even zero) convergence rate caused by the huge solution space: Theoretically, the number of possible routes between origins and destinations on a continuous surface is infinite (Zhang and Armstrong 2008).

Li, He, and Liu (2009a) modified conventional ACO to make it capable of addressing the two conflict objectives regarding cost and coverage, respectively, and exploring path over a raster surface. In their model, they used *utility*, a measurement that integrates both cost and coverage, to evaluate the optimality of a path. The exploration of path is a cell-wise process, allowing spatially continuous information required for accurately and precisely estimating the cost and coverage to be well taken and integrated. To improve the convergence rate (i.e., efficiency) of the model, they implemented a more sophisticated pheromone-updating strategy and replaced the heuristic function on visibility (η in Equation 6) with a carefully designed direction function to guide the ant's decision regarding into which neighboring cell to move. The goal of the direction function is to achieve a balance between local exploration and destination reaching. Preliminary tests on the modified ACO model have shown encouraging results (Li, He, and Liu 2009a).

Coupling the Simulation Model with the Optimization Model

Many fast-growing regions have witnessed rapid urban expansion and land use changes. In such areas, coupling land use simulation and planning optimization should greatly benefit regional or urban planning, because, for example, both the cost and the coverage of a planned road can change along with the land use changes. So far, simulation models and optimization models have been used separately in geographical applications. Particularly, although cellular automata can effectively simulate the evolution of open, nonlinear, and stochastic urban systems, to our knowledge they have not yet been used to provide inputs to urban optimization models. In this study, we explored the methodological and technical approach to coupling the CAbased land use simulation with the ACO-based path optimization under an urban setting.

The methods of model integration can be classified into two categories: loose coupling and tight coupling (Sikder 2009). For this study, loose coupling means that a simulation model interacts with an optimization model through a stable interface and that the two models do not interfere with the one another's internal implementation. We adopted the loose coupling method in this study because of its simplicity and convenience that changes in one model will not affect the other. In our integrated system, the communion between the two models is achieved through message exchange. Particularly, the various scenarios generated by the simulation serve as the inputs to the path optimization model, so that the optimization can be based on the updated information about a changing urban environment. We named our integrated system GeoSOS (available at http://www.geosimulation.cn/).

In this study, we tested two strategies for the optimization to take the simulation inputs: the piecewise strategy and the merging strategy. Under the piecewise strategy, the optimization is performed over the simulation result for a specific time point and does it for every time point under consideration. Among the multiple optimization results generated in this way, the one with the maximum optimality value is considered to be the most optimal. The merging strategy requires the simulation results for different time points to be first merged and then the optimization is performed over the merged result.

Case Study: Identifying the Optimal Path for a Planned Expressway in Dongguan, China

The Study Area

In this case study, we applied the GeoSOS to identifying an optimal path for a planned freight expressway in Dongguan, China. Dongguan is a city located in the Pearl River Delta, one of the fastest growing economic regions in China. The city consists of four urban districts and twenty-nine towns. Being about fifty miles north of Hong Kong, Dongguan's geographical location has been attractive to the manufacturing industry. In the past three decades, the area within the administrative boundary of the city has experienced a rapid transition from being largely rural to one of the world's largest manufacturing centers. For example, a single plant in Dongguan produced more than 30 percent of the world's magnetic recording heads used in hard disk drives, and another supplied 60 percent of the electronic learning devices for the U.S. market in 2005 (Chaudhuri 2009). Houjie, a town of Dongguan, is home to the largest paper-making plant in Asia.

As urbanization and industrialization have expanded in Dongguan, so have the demands on the transportation capabilities in the region (Planning Department of Dongguan 2002). Figure 1 details the transportation flows among the major industrial centers of Dongguan. As shown in this map, transportation flows are closely related to industrial activities. Although transportation demands have continued to expand during the past thirty years, the increase of the total length of expressways in Dongguan has lagged far behind its economic growth. More recently the local government has determined that the current transportation condition has become a bottleneck to maintaining Dongguan's leading position in the international manufacturing industry. To alleviate the current traffic congestion problem, the government is planning a new freight expressway that connects the eastern and western parts of the city.

The Variables and Data

As explained earlier, the objective of the ACO-based path optimization is to maximize the utility value of a path, and in regional or urban planning the utility value is typically designed to represent the trade-off between two usually conflicting factors: cost and benefit. In our specific case in Dongguan, the primary benefit considered was the new expressway's capability of meeting the transportation demand resulting from the expansion in local industrial production. We evaluated this capability by measuring the industrial activities falling into the neighborhood of the path and named it service coverage. The primary costs considered include the travel cost, which is represented by the total length of the path, and the development cost, which is determined by the land use and slope along the path. We are fully aware that in real-world transportation planning, many other important factors must be taken into account, such as environmental, social, and political factors. In this study, we chose to focus on the service coverage and

Li et al.





some basic costs of the expressway because, first, they are among the fundamental factors in transportation planning and are likely to be factors considered during the early planning stages and, second, for the purpose of exploring the methodology of coupling simulation and optimization, simplifying the scenario and focusing on those factors that can be easily represented by available data and handled by the current GIS and remote sensing technologies seems to be a reasonable strategy.

Figure 2 displays the specific variables used to generate the estimates of the service coverage and cost. The service coverage was estimated from the industrial land use distribution, which was provided by the CA simulation. The empirical land use changes that will be used as the dependent in the CA model calibration were identified by comparing the land use data layers for 2004 and 2007. These two land use layers were created through visual interpretation and manual delineation to the 0.61 m-resolution QuickBird satellite images in 2004 and 2007. Among all land use classes, the industrial land use is the one most important to this study. Thanks to its unique shape and textural information in the high-resolution images, this class can be clearly separated from other classes. Specifically, manufacturing buildings have large square shapes and a low-density distribution, whereas residential buildings are much smaller in size and have a high density (Figure 3). The data of the independents in the CA model calibration include the layers of main roads, expressways, railways, town centers, and urban district centers.

The development cost was estimated based on land use types and slope. In the land use aspect, for example, the average development cost of road construction in urban areas is much higher than that in rural areas (O'Flaherty 1967), and the cost in the water class is much higher than those in other land use classes because of the construction of bridges. In this study, we used a lookup table to translate land use type and slope gradient into their corresponding unit development costs at a cell. This lookup table was defined according to O'Flaherty's studies and the local experiences from the experts of the Planning Department



Figure 2. Spatial variables prepared from geographical information systems and remote sensing: (A) Industrial land use, (B) slope, and (C) various kinds of roads.

of Dongguan (Tables 1 and 2). The slope layer was retrieved from the digital elevation model data provided by the planning department. Figures 4A and 4B show the two cost surfaces generated in this way. The overall development cost was calculated as a simple summation of these two costs (Figure 4C).

The total size of the study area is $4,067.75 \text{ km}^2$. The computation burden would be unbearable if we



Figure 3. Provision of transport service to the rapidly growing rural industry in the Pearl River Delta. (Color figure available online.)

directly sent the raster layers at their original resolutions into the optimization model. To limit the computation to a reasonable level, we converted the resolutions of all the raster layers to 250 m. Under this resolution, there are a total of 307×212 pixels in each layer.

Model Implementation and Results

In this study, we chose to use the revised logistic CA model proposed by Li, Yang, and Liu (2008) to simulate the land use changes. The first step of this simulation was to calibrate the CA model using historical data. The empirical information about the industrial land use changes was obtained from the land use data of 2004 and 2007 (interpreted from the QuickBird images). With this empirical information as the dependent variable, the transition rules of CA were derived (i.e., the CA model is calibrated) through the logistic regression (Wu 2002; Li, Yang, and Liu 2008), using a series of proximity variables as independent variables,

 Table 1. Unit costs of road construction for various types of land use

Land use	Agricultural							
type	Water	Urban	Orchard	land	Forest	Other	Grass	
Unit cost	6	5	2	2	2	2	2	

including the distances to main roads, expressways, railways, town centers, and urban district centers. Equation 2 was then specified as follows:

$$z_{ij}^{t} = 0.871 - 0.48 x_{\text{mainroad}} - 0.06 x_{\text{expressway}} - 0.005 x_{\text{railway}} - 0.02 x_{\text{towncenter}} + 0.01 x_{\text{districtcenter}}$$
(11)

where $x_{\text{mainroads}}$, $x_{\text{expressway}}$, x_{railways} , $x_{\text{towncenter}}$, and $x_{\text{districtcenter}}$ represent the distances to main roads, expressways, railways, town centers, and urban district centers, respectively.

The calibrated CA model was validated by using a part of the training data. The validation was carried out by using a total of 10,961 cells with known land use changes from the classified remote sensing data that have not been included in establishing this model. The selection of these validating sites was based on the stratified random sampling strategy (Li, Yang, and Liu 2008). The total accuracy was 0.63 using these validation data. The validated model was then used to simulate the dynamics of industrial land based on the historical trend. When estimating the service coverage, instead of simply using a binary value to indicate whether a cell is "industrial" or not, we chose to use the industrial output value at each cell. The original industrial output value is a statistic compiled at the town level by the local government to quantify industrial activities. To get this value at each cell, the town-level value was

4-10 10-16 16-22 22-28 28-34 34-40 40-45 >45 Slope (degree) <4 Unit cost 2 2.5 3 3.5 4 4.5 5 5.5 6

 Table 2. Unit costs of road construction for various types of slope

divided by the number of simulated industrial cells within the town. A quantified industrial activity measurement like the industrial output value should be more accurate in representing the local transport de-



Figure 4. Cost surfaces related to land use and slope: (A) Cost surface from land use, (B) cost surface from slope, and (C) combined cost surface from land use and slope.

mand than the simple binary value and in turn should make the simulation more useful to the later path optimization for the planned expressway. We also used the historical town-level industrial output values to establish linear regression models by which the values for the coming years could be extrapolated. Although the immediate output from the simulation for a year was still binary (i.e., it only showed whether a cell would be an industrial one or not), with the predicted town-level industrial output values of that year, the simulation result could be quantified through disaggregation. The industrial output values of each town in 2002, 2003, 2004, 2005, 2006, and 2007 were obtained from the Statistical Yearbook of Dongguan.

To prioritize the transportation demands that are relatively distant from the existing road networks, we adjusted the industrial output value using a distance decay function as follows:

$$V^{ij'} = V_{ij} (1 - e^{-0.0003r})$$
(12)

where V_{ij} is the original industrial output value at cell (i, j), V' is the adjusted value, and r (in meters) is the distance between (i, j) and the closest existing road. The effect of this adjustment is shown in Figure 5.

We simulated the distribution of industrial land use in 2008, 2011, 2014, 2017, and 2020. Based on the simulation results, for each of the years we generated both original and adjusted industrial output value surfaces (Figure 6), as well as the cost surface. These raster surfaces were then sent into the optimization module of the GeoSOS to identify the optimal path for the planned expressway.

In this study, we revised the conventional pheromone updating strategy in ACO to incorporate both the cost and service coverage. Specifically, Equation 9 was revised as follows (adapted from Li et al. 2009a):

$$\Delta \tau^{k}(t) = \frac{Q \sum_{R(k)} V_{ij}(t)}{C_{k}(t)}$$
(13)

where $\Delta \tau^{k}(t)$ is the intensity of pheromone on the trail left by ant k when it finishes the trip from the origin





to the destination in iteration t; $\sum_{R(k)} V_{ij}(t)$ is the total industrial output value (either original or adjusted) within the buffer distance R to the trail left by ant kin iteration t, that is, the service coverage of the trail; $C_k(t)$ is the total cost of the trail; and Q, as in Equation 9, is a user-specified constant.

Based on Equations 12 and 13, we considered four different scenarios for the optimization. The first scenario is the most basic, in which V is the original industrial output value and C is the total length of the path. This scenario does not consider the influences of the existing road network and the development cost (measured based on land use and slope). In other words, it assumes that there are no existing roads and all the cells have the same development cost. The second scenario differs from the first by using the adjusted industrial output value to take into account the existing road networks. The third scenario differs from the first by incorporating the development cost. In this scenario, each cell has its unique development cost determined by local land use and slope (Figure 4), and the total cost of a path thus consists of both travel cost and development cost. The fourth scenario is a combination of the second and the third scenarios. It is the most sophisticated and arguably the most realistic of the four. As an example, Figure 7 shows the optimization results for the four scenarios based on the simulation results for 2008. Table 3 lists the parameters of the ACO model and their values used in this case study. The first five parameters were from the classical ACO and their values were set following Dorigo, Maniezzo, and Colorni (1996). The last parameter, R, which was first introduced into ACO by

Li, He, and Liu (2009a), is the buffer distance to define the neighborhood around the path within which the service is available (but declines as the distance increases).

2014, 2017, and 2020.

We evaluated the optimality of a generated path at one time point using its utility, which is calculated as follows:

$$U = \frac{\sum_{R} V_{ij}}{C}$$
(14)

Basically, the utility is the ratio between the service coverage and the total cost of the path. Note that Equations 13 and 14 are based on the same idea. The only difference is that Equation 13 is about a trail explored by an ant, and Equation 14 is about the final identified optimal path.

We evaluated the overall optimality of an identified path for the entire period under concern using the accumulative utility, which is a summation of the path's utilities for all the simulation results within the period:

$$U_{Accum} = \sum_{y=1}^{n} U_y \tag{15}$$

In our specific case, U_{γ} is the utility of the path for year y and *n* is total number of years for which the land use changes have been simulated.

We implemented both the piecewise and merging strategies described earlier for the optimization to utilize the simulation results. For the piecewise strategy, we performed optimization over the simulation results of each of the five years under simulation (2008, 2011, 2014, 2017, and 2020). We then calculated the utility value of each of the five paths for each of the five years; that is, each path received five utility values. The five utility values were then summed up to get the accumulated utility value of the path for the entire study period. For the merging strategy, we first integrated the simulated industrial output values of the five years and then performed the ACO optimization over the resulting merged surface. In this study, we merged the simulation results of the five years through simple cell-wise summation. We then, as with the piecewise strategy, calculated the utility of the identified optimal path for each of the five years and summed up the five values to obtain the accumulative utility value.

Figure 8A and Table 4 show the optimization results generated using the two strategies for the fourth scenario, the most sophisticated of the four scenarios tested, which involves both the existing road network and the spatial variation of development cost. In each column of Table 4, the highest yearly utility value occurs at the diagonal position of the table. For example, Path 2008 has the highest utility value for the simulation results for year 2008, compared with other paths' utility values for this year. This indicates that the optimization is sensitive to different simulated patterns and among all the identified paths the one generated based on one pattern is indeed the optimal one for that specific pattern. In each row of Table 4, the utility values monotonically increase over the period and this trend is consistent for all the paths. This is because the

Table 3. Parameters used in this ant colony optimization path-covering model

	•	0			
Iteration	Ants	α	β	ρ	R
2,000	20	2	2	0.1	20





Figure 7. Four scenarios of path optimization based on the industrial output value in 2008: (A) Scenario 1, (B) Scenario 2, (C) Scenario 3, and (D) Scenario 4.

simulation predicts that from year 2008 to year 2020 the industrial land use, as well as the associated industrial activities, in this area will experience rapid growth. As a result, the absolute transportation demand falling under the service coverage of the expressway will increase over the period. This understanding helps correctly interpret the values in Table 4. For example, this explains why it does not make sense to state that Path 2008 becomes more optimal in 2011 than in 2008, albeit the utility value in 2011 is 19.81 and in 2008 is 15.42. The last column of Table 4 shows the accumulative utility value of each path. The accumulative value is useful when the planner wants to evaluate the optimality of a path for a given period if the expressway is to be built at the beginning of the period. For example, although Path 2017 is generated based on the simulation result of 2017, it could still be built in 2008 and have an accumulative utility value of 154.03 over the period from 2008 to 2020. Among the five paths identified using the piecewise strategy, the one based on the simulation results for 2017 (Path 2017) has the highest accumulative utility value and thus is considered to be the best.

The bottom row of Table 4 shows the utility values of the path generated using the merging strategy (Path-Merge). Its performance in 2008 and 2011 is slightly

Table 4. Accumulative utility values based on the simulated patterns of industrial output value (V)for various years (106 RMB/km)

Optimization	Simulated patterns of industrial output value (V)							
	V 2008	V 2011	V 2014	V 2017	V 2020	Accumulative		
Path 2008	15.42	19.81	25.83	34.12	45.15	140.33		
Path 2011	15.23	20.21	26.96	36.81	50.26	149.47		
Path 2014	14.67	19.88	27.36	38.12	53.46	153.48		
Path 2017	13.32	18.75	26.85	38.87	56.24	154.03		
Path 2020	12.15	17.70	26.08	38.56	57.04	151.53		
Path Merge	14.06	19.39	27.21	38.64	55.42	154.72		



Figure 8. Optimal paths identified by coupling with urban simulation: (A) Optimal paths based on urban simulation and (B) identification of the maximum accumulative utility. (Color figure available online.)

poorer than the corresponding paths generated using the piecewise strategy (14.06 vs. 15.42 in 2008 and 19.39 vs. 19.81 in 2011) but is significantly better in the latter three years, especially in 2020 (55.42 vs. 45.15). Its accumulative utility value is greater than that of Path 2017 (154.72 vs. 154.03), the best of the five piecewise-strategy paths, indicating that the merging strategy could be advantageous over the piecewise strategy (Figure 8B).

Another important issue revealed by the data in Table 4 is that among all the identified paths the one based on the simulation results for 2008 has the lowest accumulative utility value, which means it is the least optimal path if we are considering the entire period from 2008 to 2020. Among all of the simulation results, the ones for 2008 are closest to the current situation, and this confirms one of the major suppositions that motivate this study: An optimization that is based on the current situation and assumes it to be static could have a poor performance in a fast developing region.

Conclusion

In this article we presented a methodological and technical exploration of coupling simulation with optimization to serve regional or urban planning in a fast developing region. In the simulation aspect, we chose to use the widely studied CA to simulate and predict land use changes. In the optimization aspect, we implemented a raster-based ACO method to identify the optimal path running across a real-world landscape surface. We developed two different strategies (piecewise and merging) for the ACO-based optimization to use the results of the CA-based simulation as inputs and applied the integrated system to a task of identifying optimal path for a planned expressway in Dongguan City, which is located in one of the fastest developing regions of China. In the past three decades, the area currently enclosed by the administrative boundary of the city has experienced a drastic transition from a largely rural area to an international manufacturing center. A major supposition that motivated this study is that in such an area the optimization in planning (e.g., identifying the optimal path for a planned expressway) might not be able to well serve its purpose if it assumes static land uses, as is done in most existing optimization models.

Our case study has empirically confirmed the preceding supposition and suggested that coupling simulation with optimization can considerably improve the optimality in planning. In our case study, the path identified based on the land use pattern of year 2008—the pattern that is closest to the current situation and thus the path that can be considered as a result from a noncoupling approach—has the lowest optimality value (measured by the accumulative utility) over the entire period under concern, compared with the other paths that take into account predictions for future years in one way or the other. Among all paths, the one generated with the merging strategy that combines simulation results of all the years under consideration turned out to have the highest optimality value over the entire period, although it might not always be the most optimal one for a specific single year. Particularly, in terms of the accumulative utility, the path generated with the merging strategy shows an improvement of 10.3 percent (154.72 vs. 140.33), when compared with the one from the noncoupling approach (i.e., the path based on the simulation results for year 2008). Between the two coupling strategies, in most cases the merging strategy is noticeably better than the piecewise one.

Real-world transportation planning can be very complex in the context of selecting an expressway for freight transportation. This proposed raster model did not include the distribution centers and warehouses in the path optimization because of the lack of data. Our raster method is for solving the "shortest path" problem but not the "tour problem"; that is, the method is not forcing the path to go through any given locations. On the tour problem, a raster method might be disadvantageous when compared with a vector method, and this is a topic on our future research agenda. Actually, we would treat distribution centers and warehouses the same as industrial facilities; that is, a path covering them would receive high utility values if the data are available. A raster method is advantageous in a situation that (1) besides the origin and the destination, the path doesn't "have to" go through any other locations; (2) the path needs to run through a continuously varying landscape; and (3) the path is not restricted to existing networks.

In this study we worked on specific types of simulation and optimization (CA and ACO) and applied the integrated system to a specific planning taskidentifying the optimal path for an expressway-it is clear that this approach can be expanded to other methods and applications. Indeed, a particular goal in our plan of further developing the GeoSOS is to incorporate more simulation and optimization methods so as to improve and expand its applicability. For example, it is within our immediate research interest to test the performance of agent-based modeling (ABM), another type of bottom-up approach, in an optimization-oriented planning application. ABM is effective when individual-level information is available and is considered to be flexible and intuitive for modeling certain geographical phenomena in which the accumulated impact of individual decisions leads to human-induced environmental changes (Parker et al. 2003; Li and Liu 2007). ABM is good at dealing with complex systems involving both social and natural factors (Torrens and Benenson 2005; Bennett and Tang 2006; Manson 2006; Torrens 2006; O'Sullivan 2008). Particularly in modeling land use dynamics, ABM is advantageous in incorporating various techniques, such as sample surveys, participant observation, field and laboratory experiments, companion modeling, and GIS and remotely sensed data (Robinson et al. 2007).

Another item on our future agenda is to expand the optimization functionality of the GeoSOS from path finding to facility siting and area optimization. These optimization tasks might use different optimization models and thus might require different considerations and techniques to be integrated with geo-simulations.

We argue that the idea of coupling simulation with optimization is generally meaningful to many geographical applications, and there is great potential for research in this direction. Our work could serve as an exploration to a new way of using GIS and spatial analysis in planning. More broadly, thanks to the complex and dynamic processes and relationships involved in environmental modeling, resource management, and spatial planning, GIS needs to go beyond the basic analytical capability and static data model used in most current commercial GIS packages. For almost two decades it has been noted that the data models and analysis methods provided by GIS are simply not rich enough in geographical concepts and understanding (Gahegan 1999). Moreover, it seems clear that GIS needs a strong scientific and intellectual component if they are to be any more than a commercial phenomenon (Goodchild 1992). Particularly, GIS lack the capability of simulating and analyzing the phenomena of selforganization, phase transition, and bifurcations (Batty and Longley 1994). Nowadays, this problem becomes only more obvious and urgent (An et al. 2005), and to address it is the aim of this study and its subsequent work.

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