Towards an *in silico* Experimental Platform for Air Quality: Houston, TX as a Case Study

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Abstract. In this paper we couple a spatiotemporal air quality model of ozone concentration levels with the synthetic information model of the Houston Metropolitan Area. While traditional approaches often aggregate the population, activities, or concentration levels of the pollutant across space and/or time, we utilize high performance computing and statistical learning tools to maintain the granularity of the data, allowing us to attach specific exposure levels to the synthetic individuals based on the exact time of day and geolocation of the activity. We demonstrate that maintaining the granularity of the data is critical to more accurately reflect the heterogeneous exposure levels of the population across time within the greater Houston area. We find that individuals in the same zip code, neighborhood, block, and even household have varying levels of exposure depending on their activity patterns throughout the day.

Keywords: synthetic populations; air quality; ozone; personal exposure

1 Introduction

It has been demonstrated that localized specific exposures to ozone can dramatically increase health risks for cardiac events and asthma [4, 5, 20]. For example, it was found that an increase of 20 parts per billion (ppb) in ozone (O_3) over a period of one to three hours is associated with a 4.4% increased risk of having an out-of-hospital cardiac arrest, for which 90% of cases result in death [4]. Many studies, however, use 12- or 24-hour activity summaries [10, 12, 16]. However, aggregating time to daily periods miss important details such as variations in ozone levels across physical space and time, which can significantly impact individual and population exposure levels to ozone.

In this paper, we couple a spatiotemporal air quality model of ozone concentration levels (O_3 ppb hourly) across the metropolitan area of Houston, Texas to a data-informed synthetic information model. It overcomes the limitations of traditional approaches as it is informed by how people move through their activities during the day, allowing us to attach specific exposure levels to the synthetic individuals based on the exact geolocation of the activity and time of day. The result is a step towards an *in silico* experimental platform to study social behavior, including interaction with the environment. While previous models have calculated personal exposure, the space and time coupling makes this model unique. In addition, earlier models often aggregated exposure levels to calculate a population exposure, but computational resources have given us the ability to maintain the granularity of the data at the individual level across both space and time. Our contribution is the adoption of the synthetic information approach to understand the impact of air quality over physical space and time on individual exposure levels. This requires a richer characterization of the synthetic individuals and their activity sequences than in current models. We demonstrate that maintaining the granularity of the data is critical to more accurately reflect the heterogeneous exposure levels of the population within the Houston Metropolitan Area. We find that individuals in the same zip code, neighborhood, block, and even household have varying levels of exposure depending on their activity patterns throughout the day.

2 Background

Exposure is the contact an individual has with a pollutant, and is a function of the concentration of the pollutant and the time exposed to the pollutant [25]. An individual's exposure has often been assumed to be proportional to the ambient concentration of the air pollutant. However, an individual's activity patterns across both space and time must be accounted for in order to determine a more accurate representation of the magnitude, frequency, and the duration of individual's exposure to a pollutant [29].

Community-based studies [21, 23, 31] identify a significant impact on health from air pollution levels but do not directly measure individual exposure. Other studies focus on direct measurement of human exposure through personal monitors or home-based centers, but the cost, measurement accuracy, and logistics limit their use on a scale large enough to provide community-wide understanding of exposure [30, 28]. Earlier models that sought to attach air pollution exposure to populations, took a group-level approach, whether based on the demographics of a subset of individuals, the geographic location of homes and activities, or a set of micro-environments. While some of these studies modeled representative individuals [11, 2, 19], they either stopped short in their ability to trace individuals throughout the course of the day or in modeling a representative population of the geographic location in question. For instance, a variety of Environmental Protection Agency (EPA) exposure models (e.g., APEX [26] and SHEDS [27]) utilize the Consolidated Human Activity Database, a repository of harmonized human activity data. In this database, a person's exposure is obtained by mapping the activities reported in the surveys into several micro-environment categories, each with an estimated exposure rate. In contrast, we will map the reported activities to very granular geolocations accounting for the time of day. Other exposure models have focused on calculating personal exposure to emissions and other pollutants while traveling, accounting for factors such as transportation mode, vehicle type, and transportation routes [7, 9]. While these models seek to accurately reflect exposure during travel, they do not account for the individual's full course of activities.

Moving away from aggregate-level exposure calculations and accounting for an individual's full course of activities, more recent exposure models have developed synthetic populations to represent each individual in a geographic location. Traditional synthetic population models, however, are limited in their use for estimating environmental exposure to contaminants that vary over both space and time. These methods aggregate activities into percent time (e.g., percent of day) and allocate the aggregated time to an activity location [13, 17, 32]. Coupling these models to environmental exposure will mask important social determinants of health. As an example, a study of Sydney, Australia [18] used traditional models with single daily exposure values, and coupled the percent time spent at various locations to these daily average exposure levels. However, that level of granularity is not enough for differentiating important health effects related to air quality. In contrast to this study, our research attaches actual exposure values to the synthetic individuals continuously over space and time, i.e., at specific geographic locations and specific points in time. It has been shown in many studies [4, 5, 20] that level of aggregation is an important consideration as it can mask important health effects that could be translated into life saving behavioral and policy changes.

Developing an *in silico* experimental platform will allow us to study disparities in exposure to air pollution at a level of detail not possible with other models. This level of granularity will improve our understanding of the exposure pattern differences for sensitive and socioeconomically disadvantaged subpopulations compared to the population at-large. The *in silico* platform will enable more in-depth analysis than is currently possible with existing approaches of populations at risk of environmental exposure (air quality).

3 Methodology

In this section we describe the current state of development of the *in silico* experimental platform, a platform that couples a synthetic information representation of the residents in the Houston Metropolitan Area to an air quality spatiotemporal model. We begin by describing the synthetic information model developed at Virginia Tech [15] in Section 3.1. It includes socio-demographically relevant activity sequences and the movement of each individual in the population through their sequences second-by-second during the day. This allows aggregation of time intervals to match the environmental quality data (e.g., hourly intervals), which is explained in Section 3.2. Finally, we demonstrate the methodology to determine spatiotemporal individual-level exposure to ozone in Section 3.3. This *in silico* platform provides the exposure profiles for the roughly 4.9 million synthetic individuals in the Houston Metropolitan Area. Figure 1 illustrates the conceptual model of the current state of the *in silico* experimental platform. This platform will provide an integrated database that can be used and reused for the analysis of various studies related to the synthetic population and air quality.

3.1 Synthetic population information model

The first step in creating the *in silico* experimental platform is to generate a synthetic population of the Houston Metropolitan Area. The synthetic information is a set of synthetic people and households located geographically, each associated with demographic variables. It is created by integrating a variety of databases from commercial and public sources, including statistical surveys, administrative data, and data on the built environment (e.g., buildings, roads, and land use), through a process that preserves the confidentiality of the individuals in the original data sets, yet produces realistic attributes and demographics for synthetic individuals.

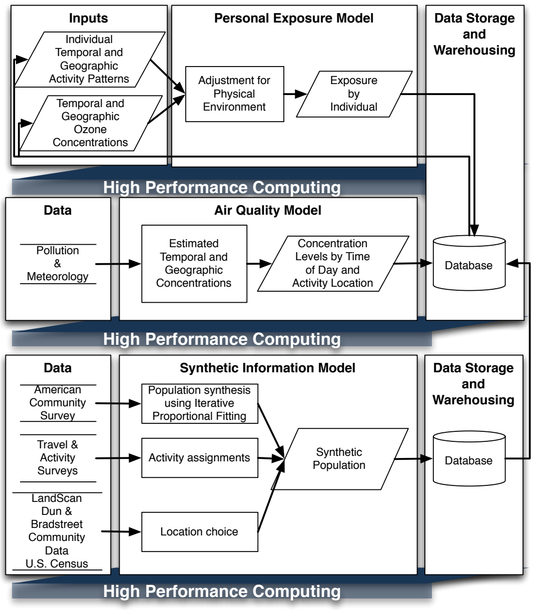


Fig. 1. Conceptual model of the current state of the *in silico* experimental platform. The bottom layer represents the synthetic information model, the middle layer represents the air quality model, and the top layer represents the personal exposure model.

The steps to this synthetic information generation include (1) population synthesis, in which a synthetic representation of each individual and household in a region is created using socioeconomic characteristics from census data, (2) activity assignments, in which each synthetic person in a household is assigned a set of activities to perform during the day, along with start and end times based on activity or time-use survey data; and (3) location choice, in which an appropriate real location is chosen for each activity for every synthetic person based on data sources, such as land use patterns, tax data, or commercial location data. The data sources used in the creation of the Houston synthetic population are given in Table 1.

The American Community Survey (ACS) provides tables of distributions on demographic characteristics, such as age, gender, household income, and household size, which are referred to as marginal distributions. Joint demographic distributions are reconstructed from these marginal distributions using an iterative proportional fitting technique [1]. The process ensures that the synthetic

Table 1. Houston Metropolitan Area synthetic information data sources.

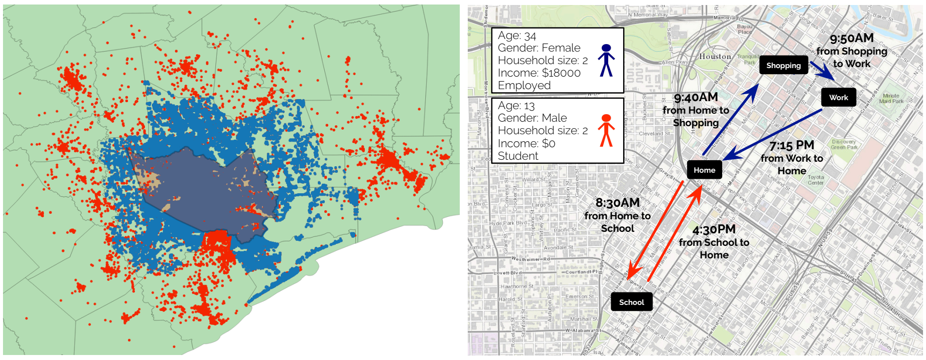
Data Source	Description
US Census TIGER Data	True population geographic boundaries and demographics to be matched by synthetic population.
US Census American Community Survey (ACS) (2005 to 2009)	Primary source of data used to build the synthetic set of people with the aggregate statistics matching US Census marginals.
National Household Travel Survey (NHTS)	Data on travel behavior and activity sequences.
Dun & Bradstreet (D&B)	Describes home locations and retail locations - used to locate activities.
HERE (formerly NAVTEQ)	Road Network and transportation map.
National Center for Education Statistics (NCES)/	Data on school locations.

population matches the marginals of the true population. Furthermore, because the distribution of the various demographic variables are generated from the ACS they are ensured to be representative of the true population. Synthetic individuals are placed in a household with other synthetic individuals. Each household is then located geographically using land-use data and data pertaining to businesses and transportation networks. Realistic activity patterns and their locations are then added. A set of activities for an average day is determined by analyzing the activity patterns in the National Household Travel Survey and linking these patterns to the socio-demographic composition of the households and individuals within the households.

The Houston Metropolitan Area synthetic population was extracted from a synthetic population developed for the entire state of Texas. Any synthetic individual with either a home or activity location within Harris County, TX was included. This resulted in approximately 4.9 million individuals grouped into 1.8 million households. Synthetic individuals can perform up to 6 different types of activities including travel; activity types can be performed multiple times by the same individual on the same day. Activities occur in 1.2 million different activity locations (895 thousand housing locations, 166 thousand work locations, 37 thousand shopping locations, 4 thousand schools, and 112 thousand other locations). Figure 2 shows the household and activity locations across the region, as well as an example set of activities for one household.

3.2 The air quality model

According to the Texas Commission on Environmental Quality (TCEQ), the air quality in Houston, TX is monitored more closely and analyzed with more intensity than perhaps anywhere in the country — if not in the world [24]. The Houston area has an extensive air monitoring network including 47 monitors measuring ozone. Monitor data, extending back more than tens years at some locations, are collected hourly using EPA federal reference methods [26] and validated by TCEQ. One hour ambient meteorological (temperature, relative humidity, and wind speed) data are available through the monitors. For this



(a) (b)

Fig. 2. Activity Locations. (a) The red points represent the 1.2 million activity locations for the synthetic population and the blue points represent the 895 thousand housing locations. The shadow is the boundary of Harris County, Texas. (b) A "close-up" of the activity patterns on an average day for a two-person household.

initial model, hourly recordings on August 26, 2008, of ozone concentration levels (O_3 ppb hourly) across 39 EPA monitors in the Houston Metropolitan Area were used.

The first step to coupling the environmental pollutant data with the synthetic information is to assign the hourly ozone concentration to each activity location (e.g., home, work, school, shopping, travel). This was done using the inverse weighted distance from each location to the 39 monitors, a standard method for assigning ozone concentration [8, 14, 22]. Given that $m_j(t)$ is the concentration measured by monitor $j \in \{1, ..., n\}$ at time t, the pollutant concentration c_i at each activity location i at time $t \in \{1, ..., 24\}$ is calculated as follows:

$$c_i(t) = \sum_{j=1}^{n} \frac{\frac{1}{d_{ij}^2} m_j(t)}{\sum_{j=1}^{n} \frac{1}{d_{ij}^2}}, \tag{1}$$

where d_{ij} is the great circle distance between location i and monitor j. Using the geo-coordinates (i.e., latitude and longitude) of the monitoring stations and the activity locations, d_{ij} is calculated as follows:

$$d_{ij} = r * arccos(sin\phi_1 sin\phi_2 + cos\phi_1 cos\phi_2 cos(|\lambda_2 - \lambda_1|)), \tag{2}$$

where $\phi_1\lambda_1$ and $\phi_2\lambda_2$ are the latitudes and longitude, respectively, of points 1 and 2 and r is the Earth's mean radius. The result is a q x p matrix, where q is the number of activity locations (approximately 1.2 million) and p is the number of hours in a day (24). At this point, each activity location for each hour of the day has an assigned ozone concentration level.

3.3 The personal exposure model

The representative day and corresponding activity sequences of each synthetic entity is linked in space and time to the corresponding ozone concentration levels.

The personal exposure model is developed by coupling the air quality model with the individual activity patterns from the synthetic information. Exposure to a pollutant is a function of the concentration of that pollutant and time. Because we are modeling each day using discrete time steps (i.e., in units of seconds), the personal exposure e_{ip} for an individual synthetic person p at a visited activity location i during the 24-hour sequence (86,400 seconds) is calculated as follows:

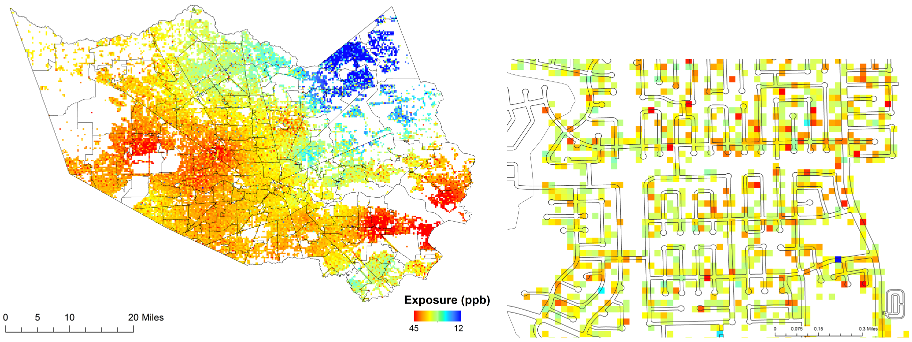
$$e_{ip} = \sum_{t_l < t_k} c_i(t_l)[t_k - t_l], \tag{3}$$

where $c_i(t_l)$ is the concentration at activity location i at time t_l and $t_k - t_l$ is the time person p spent at location i. We calculate e_{ip} for all activity locations visited by person p during the day. Note that some activity locations may be revisited at different times in the same day (e.g., home). The assignment of exposure to travel is made by splitting the travel time between the origin and destination activity locations. Therefore, travel exposure is calculated based on the concentration of ozone at the origin and destination activity locations during the time of travel.

4 Results

Previous studies have assumed that an individual's location remains the same throughout the day (i.e., individuals stay home) or have used 24-hour aggregate pollutant concentration levels (see section 2). In the model presented here, we use geolocated hourly levels of ozone concentration and allow individuals to move through their time-sequenced activities. We find that exposure levels can be quite different across Houston and even within neighborhoods and households. The cumulative exposure distribution across the entire synthetic population with homes in Harris County is shown in Figure 3, as well as a "close-up" for a single neighborhood. This demonstrates that there is heterogeneity in exposure levels within neighborhoods due to the fact that people move around during the day. The platform also allows us to trace individuals over the course of the day. Hourly exposure traces for two synthetic families are given in Figure 4. These are two demographically similar families located in different parts of Houston. This demonstrates that ozone exposure is heterogeneous even within household, illustrating the significance of our research.

As has been shown in previous studies, increases in ozone levels over the course of a few hours can have major health implications (see section 1), supporting the need for exposure calculations that are sufficiently granular. To see the impact that modeling at different levels of resolution has on population exposure, three scenarios are compared. Scenario 1 calculates exposure by using 24-hour aggregate concentration and assumes individuals stay home all day. Scenario 2 calculates exposure by using the geolocated hourly concentration levels and assumes individuals stay at home all day. Scenario 3 uses the geolocated hourly concentrations for all of the activity sites and moves the individuals through their time activity sequences for the day. This is the most realistic scenario, as it calculates exposure according to where people are physically located throughout the day. Figure 5 gives the exposure traces for the synthetic population in an area of Houston for one day using these scenarios. This demonstrates that time sensitive exposures can be quite off when not accounting for actual activity locations. While Scenarios 2 and 3 show similar patterns, Scenario 2 does not capture the extreme values. Without the level of spatiotemporal resolution of Scenario 3 we would not be able to capture the full spread of exposure, which could be particularly important if these extreme values are experienced by the sensitive population of Houston.



(a) (b)

Fig. 3. The cumulative exposure distributions for the synthetic population for August 26, 2008. (a) Shows the synthetic residents of Harris County. (b) A “close-up” of the cumulative exposure for one neighborhood.

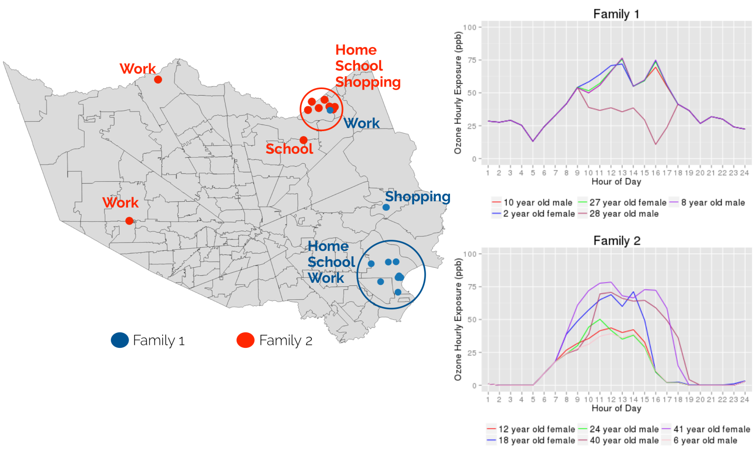
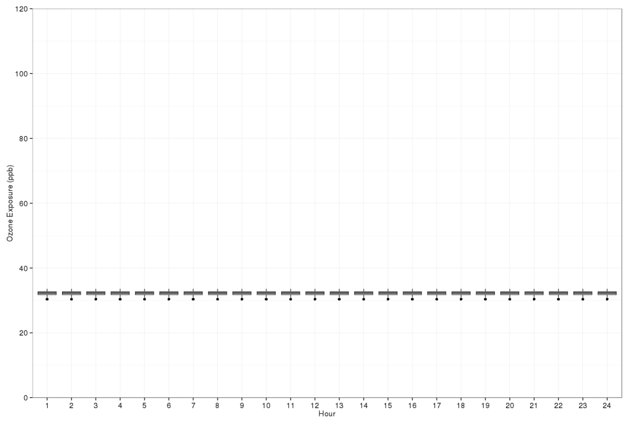
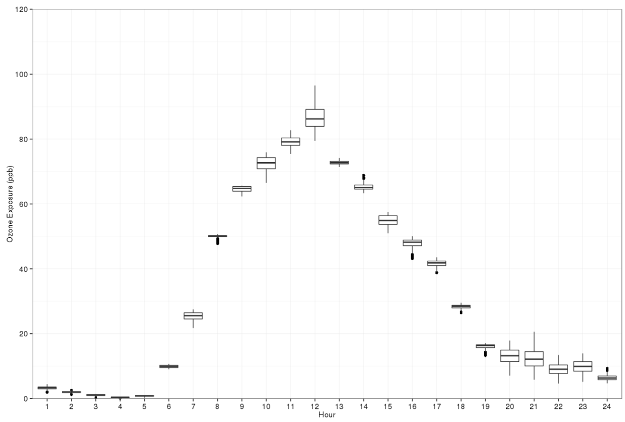


Fig. 4. Exposure traces for two synthetic families located in different parts of Houston on August 26, 2008.



(a)



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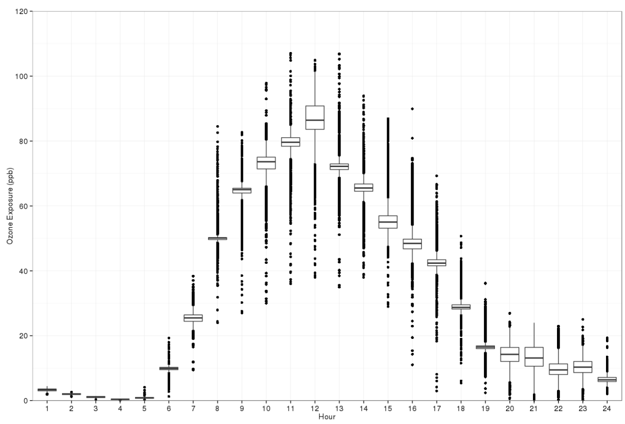

(c)

Fig. 5. Hourly exposures for the synthetic population in zip code 77026 in Houston calculated according to three scenarios, using ozone levels on August 26, 2008. (a) Scenario 1 assumes 24-hour aggregate concentrations and individuals stay home. (b) Scenario 2 allows geolocated concentrations to vary hourly and assumes individuals stay home. (c) Scenario 3 allows geolocated concentrations to vary hourly and assumes individuals move through their time-sequenced activities.

5 Conclusion

In this paper, we coupled an air quality spatiotemporal model to the synthetic information model of the Houston Metropolitan Area that captures the detailed individual-level activities throughout the day. This allowed us to attach specific exposure levels to the synthetic individuals based on the exact time of day, the geolocation of the activity, and the condition of the physical environment. This is crucial to better understanding exposure pattern heterogeneity. Models that do not account for this level of granularity in space and time would be missing important differences in the distribution of exposure in the population and within neighborhoods, blocks, and even households.

In further work, we will couple the synthetic information to an improved spatiotemporal ozone model developed by Ensor [3], which fully incorporates meteorology and provides estimates of ambient ozone levels continuously in space and time. In addition, we will extend the model to different geographic areas, beginning with the Washington, DC metropolitan area. For each region, we will create a richer representation of the synthetic information model to capture key features relevant to the social determinants of health and life style choices. We will expand the socioeconomic representations of the individuals, such as educational attainment, occupation, and health insurance status, and their associated set of activities that has relevance with respect to environmental exposure levels, such as transportation mode, transportation route, and type of day (e.g., weekday versus weekend). Moreover, we will further characterize the condition of activity locations to model ambient air quality transfer to indoor spaces, with a focus on housing or building quality, sources of heating, building occupancy, and land use (e.g., green space). Furthermore, we will generate multiple replications of the synthetic populations in order to better capture uncertainty across many runs of the model. Finally, we will test potential intervention strategies by conducting "what if" scenarios to inform policy. The platform will allow us to explore the complex interplay of policies and incentive programs related to air quality. Adjusting behavior of the synthetic population in response to a policy or program proposal will generate new estimates of exposures that can be used to compare to the original exposures. This will allow us to study policy alternatives that aim to reduce time spent outside, such as the increase in the access of public transportation, and more focused health alerts on bad ozone days. Moreover, it will allow us to explore different individual behaviors in compliance with incentive schemes based on individual characteristics, such as bus ticket vouchers for disadvantaged populations in areas identified as high risk for ozone exposure.

The coupling of improved spatiotemporal air quality models with enhanced synthetic information models will result in an *in silico* experimental platform to study disparities in exposure to air pollution at a level of detail not possible with other models. This level of granularity in the estimation of environmental exposure will improve our understanding of the exposure pattern differences, particularly for sensitive and socioeconomically disadvantaged subpopulations.

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