Identifying Unexpected Behaviors of Agent-based Models through Spatial Plots and Heat Maps*

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Abstract

Verification and validation (V&V) techniques commonly require modelers to collect and statistically analyze large amounts of data which require specific methods for ordering, filtering, or converting data points. Modelers need simple, intuitive, and efficient techniques for gaining insight into unexpected behaviors to help in determining if these behaviors are errors or if they are artifacts resulting from the model's specifications. We present an approach to begin addressing this need by applying heat maps and spatial plots to visually observe unexpected behaviors within agent-based models. Our approach requires the modeler to specify hypotheses about expected model behavior. Agent level outputs of interest are then used to create graphical displays to visually test the hypotheses. Visual identification of unexpected behaviors can direct focus for additional V&V efforts and inform the selection process of follow-on V&V techniques. We apply our approach to a model of obesity.

Keywords: verification and validation, heat map, spatial plot, visualization, agent-based models

1 Introduction

The macro level behaviors that a given agent-based model (ABM) is intended to recreate may be well understood but the mechanisms that lead to these behaviors may not be known [3, 30]. Simultaneously, some expected behaviors and types of interactions among the agents within that system may also be known or assumed to be understood. However, the modeler may face (1) incorrect, incomplete, or contradictory knowledge about the system; (2) disagreement among the model's stakeholders on how to address the problem or over which problem to solve [19]; (3) challenges resulting from conflicting model

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characteristics [18]; (4) challenges resulting from simplifying the set of allowable agent behaviors into a finite set for implementation and execution; (5) challenges in examining the combinations and sequences of events that lead to various system level outcomes [11]; and (6) challenges due to behaviors of model components changing over time [25]. Therefore, an ABM serves as a theory tester to see if the agent and environment specifications produce any *unexpected behaviors*.

Unexpected behaviors are model outcomes that cannot be explained by the model's specifications and do not pass the selected V&V techniques, such as making comparisons against trusted simulations in the same application domain, data sets from physical experiments, or subject matter experts' (SMEs) opinions [30]. It is the modeler's duty to determine if any of these behaviors represent errors within the model. Ultimately, these unexpected behaviors require understanding and explanation to determine if the behavior is an error or new knowledge in the application domain [1]. However, as an initial step, the occurrences of these behaviors first need to be identifiable from simulations' executions.

Verifying and validating unexpected behaviors requires accumulation of insight and understanding into the behaviors and the conditions under which the behaviors arise. An unexpected behavior either becomes part of a set of behaviors one considers valid or it is deemed invalid. Visual V&V methods can assist in identifying unexpected behaviors by reframing the simulation execution into a variety of different views. Each view can be tailored for the intended audience such as the modelers, the model's stakeholders, and subject matter experts at varied levels of expertise based on their perceived level of knowledge about the modeled system. Effective visualizations can help to identify, communicate, and understand important behavior from the model while facilitating insight through the detection of key features within the output [15, 26, 27]. A survey conducted on simulation modelers found that the most common approach for verifying ABMs was through visual inspection with over one third of the respondents utilizing this approach [21].

Visualization can assist the modeler in providing clearer pictures on how and why the simulation is behaving in expected or unexpected ways and also assist in conveying these finding to interested parties. To this end, we present a technique for exploring the evolving conditions within an ABM through the use of spatial plots to examine agent positions and distributions and heat maps to examine agent density statistics. We provide a use case of an ABM to illustrate our technique.

2 Background

Visualization enhances the experience of model execution by graphically representing parameter levels, distributions of values, network relationships, and interdependencies [34]. This is accomplished in part by the ability to place the simulation into context by co-locating different types of data to facilitate exploration or gathering explanations within the simulation [29]. Visual techniques provide numerous opportunities for V&V of ABMs during execution. Animation, for instance, provides the modeler the ability to observe how the system functions and helps to communicate results [23]. Data can be displayed through information visualization to gather insight through a number of graphical techniques. Some of the more commonly used techniques include scatter plots, line plots, histograms, box plots [25], bar charts, icon-based displays, dense pixel displays, stacked displays [13], data maps, time-series plots [10, 32], polar diagrams [26] and cluster heat maps [35]. These techniques utilize datasets dependent upon size, type, or dimensionality for creating visual representations [13].

Agent-based models are prime candidates to use spatial plots and heat maps as an analytic tool. Heat maps commonly assist in visualizing spreadsheets, data sets, and matrices [4] and are easily extendable to for displaying the locations of agents or environmental objects as well as clearly conveying areas where agent groupings are occurring. Heat maps can represent interactions between agents with respect to geographic location (where x and y coordinates make up the x and y axis of the heat map) or use the agent types to form the x and y axis and utilizing the color scheme to represent interactions. The heat map representations allow for a simple and easy method for detecting if agents move through areas that they are not supposed to move through due to the model specifications. It also identifies interactions or communications between agents that are not allowed to interact. Similarly, it allows the modeler to observe if any expected communications or interactions do not occur.

Visualizations convey information about the simulation; as such, it is important that the selected visualizations do not distort the representation of model outcomes and decrease the usefulness of the model [5, 10]. When incorporating visual components for V&V, several challenges exist for visualizing model results, including representing model components, representing the magnitude of changes, and poor visualization choices adding an additional level of complexity to the model [33]. These challenges specifically apply to ABMs in the following ways:

- Challenge with misrepresenting model components: Showing agent locations without any additional information does not necessarily convey how or why the group formed. Visualizations that also convey internal agent attributes, such as age or movement behavior, can provide a more accurate view of what is happening to cause the grouping behaviors.

- Challenge with representing the magnitude of model changes: Visualizations based on altering agents' representative colors and local min/max provide the illusion that a min/max value always occurs during execution; however, this does not necessarily mean that an absolute min/max value occurred.

- Challenge with model complexity: Using the same colors, icons, or shapes for different elements within the visualization or using different time scales or metrics between visual elements make it difficult to interpret the results.

Technical challenges are also important for visualizing simulations, including usability, scalability, and integrated analysis of heterogeneous data [16]. Usability refers to designing visualizations that successfully contribute to the advancement and use of visualization research. The modeler is responsible for creating a visualization that model users can easily understand. Scalability refers to how well visualization tools apply to representing large data sets. In this case, too many overlapping representations within a single view area become indecipherable and fail to convey useful information. Integrated analysis of heterogeneous data deals with visualizing data obtained from various locations in various formats. All of the data being visualized needs to be clearly conveyed for each visualization and any differences in scale or magnitude should be explicitly stated.

We can potentially improve identification of unexpected behaviors by visualizing different perspectives of the same information. For instance, visualization of the spatial distribution of an agent population as an x-y plot, as a density function, or through their movement patterns can aid analysis. This provides an extra level of insight into the model's behavior and can help a wider variety of model users or stakeholder to get a better grasp of what the simulation does. However, the creation of multiple types of visualizations may require the collection of a greater amount of data that is periodically collected throughout the simulation runtime. This entails conducting *trace validation* which focuses on examining micro-level occurrences within a model to reveal errors [2]. Traces provide the behavior of agents or the model over time to determine if the logic is correct and the simulation produces believable values [9, 11, 14]. However, the large volumes of data created through trace validation is difficult to analyze and can be burdensome to interpret [6, 36].

There have been several efforts to provide SMEs with an interface to collect, analyze, and interpret traces. [36] present a validation process for analyzing a natural organic matter model by using traces, graphs, charts, and model-to-model comparisons. Graphical charts test if the produced data curves match the expected distribution curves. This approach is suitable for inspecting the validation of population level statistics. [8] provide a V&V Calculator for examining trace data and providing a statistical measure of model characteristics that are likely contributors to various model behaviors. [6] use the Geamas Virtual Laboratory (GVL) tool to collect traces of a biomass ABM for analyzing animal wastes management. These traces collect (1) sets of messages exchanged between agents, or (2) a historical accounting of simulation execution per agent or group of agents. Visualization tools inspect these traces and identify interactions that lead to successful agent negotiations. Their visualization tool filters traces based on specific agents or characteristics. However, the GVL tool becomes unwieldy for analysis of traces once exceeding several dozen agents.

3 Methodology

Our methodology assumes that a simulation exists and is suspected to be correct. We propose a five-step approach for exploring the simulation for unexpected behaviors as shown in Fig. 1. Step 1 requires creating hypotheses, specifications, and boundary conditions for establishing baselines for determining if outcomes appear unexpected. Step 2 involves identifying outputs of interest; i.e. the outputs required to check the hypotheses, specifications, and boundary conditions identified in Step 1. Step 3 involves running the simulation. Step 4 involves collecting the outputs of interest identified in Step 2 from the simulation runs. Step 5 involves creating visual representations of the outputs of interest in order to provide a means for exploring the outcomes. These visualizations are compared against the V&V hypotheses, specifications, and boundary conditions from Step 1 to identify any suspicious behaviors. We use visualization techniques in the form of spatial plots and heat maps to conduct V&V on the simulation.

Spatial plots represent agent locations based on their X-Y coordinates. Heat maps are two-dimensional data matrices that assign color values to each point in the matrix [35]. Higher values on the heat map display at different colors than the lower values in order to visually present the difference in values across the heat map's surface. We create heat maps using the exact dimensions as the agents' environment and simply count the quantity of interest at a particular location on the grid. A smoothing function is applied

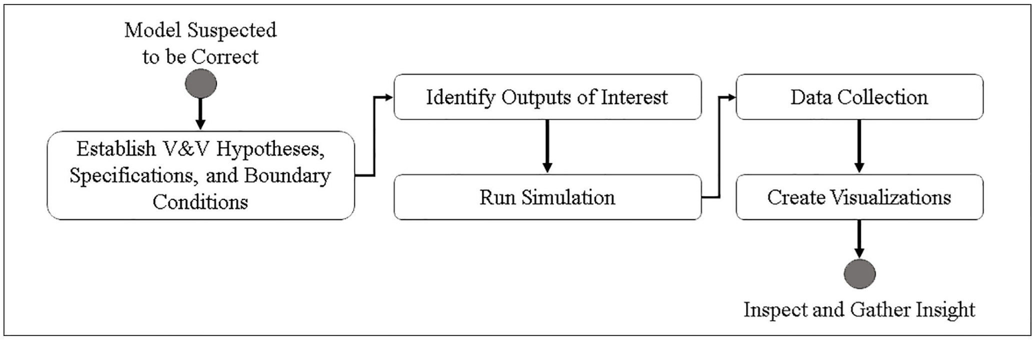


Figure 1: Methodology for visually identifying unexpected behaviors of ABMs to gather insight

while transitioning from the high values matrix cells to the lower value adjacent cells. The smoothing function ensures color continuity; thus, improving the viewer's experience.

We utilize these visual methods to identify unexpected behaviors by reframing the simulation execution into a variety of different views, such as agent locations, movement patterns, or agent attribute values distributed across the environment to name a few. Each of these views can be tailored for the intended audience based on their prior knowledge of the system. To collect the micro-level data needed to identify errors we apply trace validation and store agent locations and parameter values over time. Then we create spatial plots to examine agent positions with respect to the environmental dimensions. We explore and examine population statistics and their distribution across the environment by creating heat maps.

4 Use Case: Obesity Simulation

We apply our methodology to inspect a simulation of obesity comprised of a society represented by a combination of individuals and environmental factors. We develop our model by first establishing a set of base assumptions and constraints to illuminate expected outcomes and boundary conditions for our obesity system following the Modeling and Simulation - System Development Framework [31].

4.1 Model Details

This is a simplified version of the Obesity Model described in [28], [17], and [8] in which we focus exclusively on weight gain of individuals due to their access to food within their environment. The model consists of four agent populations: *people*, *homes*, *restaurants*, and *workplaces*. People have three possible eating habits: low, medium, or high calorie. They eat three meals a day at fast food, markets, and non-fast food restaurants [20, 22]. The number of calories gained from each meal is dependent upon the person's eating habit along with the restaurant type. The basal metabolic rate (BMR) equations capture the weekly calorie requirements for maintaining a person's current weight [12, 24] as shown in equations 1 and 2 (with Weight in pounds, Height in inches, Age in years, and BMR in calories).

$$BMR_{male} : 88.362 + (29.535 * Weight) + (1.889 * Height) - (5.677 * Age) \quad (1)$$

$$BMR_{female} : 447.593 + (20.386 * Weight) + (1.219 * Height) - (4.330 * Age) \quad (2)$$

The remainder of our core assumptions and constraints that form our model:

- *People* have age, height, weight, and gender attributes in order to use Body Mass Index (BMI) to classify as Obese (BMI $\geq$ 30), Overweight (30 $>$ BMI $\geq$ 25), Normal (25 $>$ BMI $\geq$ 18.5), and Underweight (BMI $<$ 18.5).
- *People* (1,000 created), *Homes* (100 created), *Workplaces* (100 created), and *Restaurants* (100 created) are uniformly distributed throughout the environment.
- The environment is a 625 x 625 unitless grid.
- Each person is assigned one *home* and one *workplace* at random.
- There is no limit on the number of people that can be assigned to a *home* or *workplace*.
- Starting age, weight, and height are specified by the user, but all *people* are at least 18 years old.
- *People* move from their home to their work, and back to their home (exclusively in this order) every day.
  - One meal is obtained at each location each day for a total of three meals.
  - To obtain a meal, each person selects a restaurant within 30 units of their current location at random.
  - Calories are determined based on the restaurant selected combined with the person's eating habit.
  - Calorie gain accumulates over the course of a week for each person.
- Restaurants produce a calorie amount for each meal based on the restaurant's type:
  - 400-900 calories per meal from Market type.
  - 600-1100 calories per meal from Non-Fast Food type.
  - 800-1500 calories per meal from Fast Food type.
- Eating habits modify the allowable calorie gain from each meal:
  - Low-Calorie eating habit pulls samples from the bottom 50% of the restaurant's calorie range.
  - Medium-Calorie eating habit samples within the 25%-75% (middle) of the restaurant's calorie range.
  - High-Calorie eating habit samples from the top 50% of the restaurant's calorie range.

- People update their weights at the end of each week based on the difference (positive or negative) between their calories consumed that week and their current BMR value.
- Calorie gain resets to 0 each week and the obesity status of each individual is tracked over time.

We formulated two hypotheses to drive the selection of assumptions and constraints: (1) we hypothesize that the home and work locations of the people agents affect the growth of obesity over 15 years due to their proximity to different types of restaurants; and (2) we hypothesize that eating habits affect the growth of obesity over 15 years.

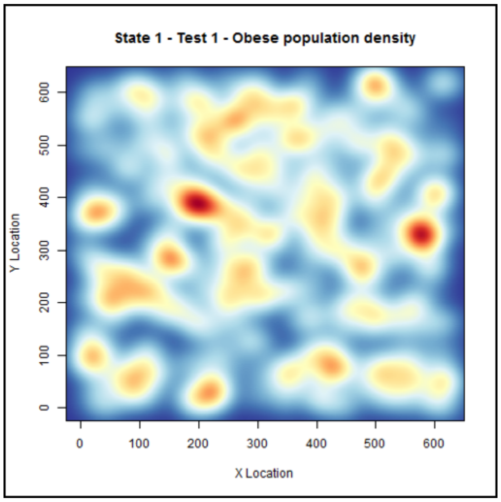
4.2 Experimentation

Creating spatial plots and heat maps of our outputs allows us to verify that the assumptions and constraints connected to the test cases are not violated and to conduct an initial validation of our two hypotheses. We utilize these visualizations to conduct a quick, visual search into the model's behaviors to identify obvious errors (such as an agent appearing outside of the expected 625x625 grid) while receiving intuitively analyzable feedback on what is happening within the simulation and what contributing factors appear to be supporting these happenings. We use the visualizations to gain insight into the model which can then assist the modeler in identifying next steps for additional verification and validation exercises. Note that while we display visualizations on the results of single runs to convey our approach, replications remain necessary for proper testing and each replication requires its own set of visualizations.

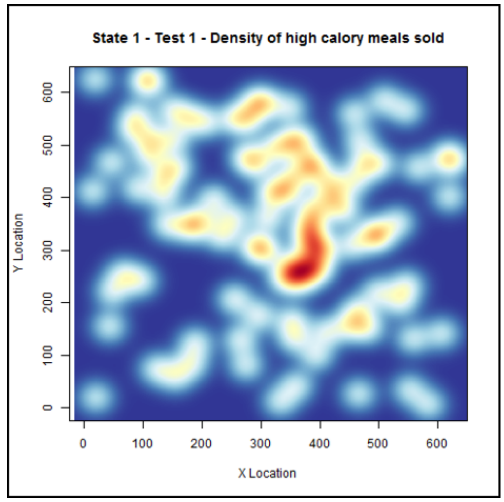
Hypothesis 1 suggests several items that we want to check within the simulation. On the verification side, we want to ensure that (1) all agent populations appear to be uniformly distributed within the 625x625 environment, (2) that no agents move outside the bounds of the environment, and (3) that people move between homes and workplaces every day. To assess the validity of our hypothesis, we identify the following outputs of interest:

- The number of calories that each person gains from each restaurant per meal;
- The location of each person's home and workplace;
- The location and type of each restaurant that the person visits per meal;
- Each person's weight/BMI classification over time.

We run the test case for 15 years of simulation time and collect the outcomes of interests for each agent. For this experiment, we equally distribute the three eating habits throughout the People population. We then create spatial plots to visually inspect the three verification items of interest by (V1) plotting each agents position within a spatial plot, (V2) plotting only agents which appear outside of the environment grid, and (V3) plotting People agents whose positions do not change throughout the day or whose end of day positions differs from their start of day positions. These three visualizations do not reveal any unexpected behaviors. The spatial plots for V1 appear uniformly distributed (at minimum they lack the appearance of large agent clusters) as expected and the plots for V2 and V3 are blank (indicating no violations occurring within the first test case).



(a) Density of people classified as obese.



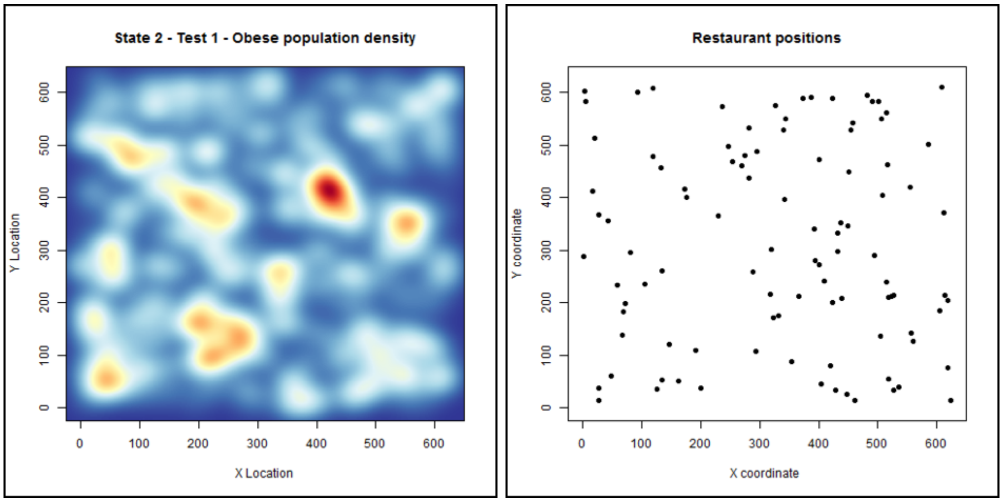
(b) Density of high calorie meals sold.

(c) Color scale.

Figure 2: Test case 1

We then create heat maps to spatially represent the weight density of people agents and density of high-calorie meals sold, as depicted in Fig. 2(a) and Fig. 2(b). To create Fig. 2(a), we count the number of People at each coordinate with each BMI classification using both home and workplace locations. Then, we compute the density of the obese population based on the number of people living in each home and working at each workplace. For Fig. 2(b), we plot heat map of high-calorie meals sold within the environment to reveal the locations where people with high-calorie eating habits are eating. Fig. 2(c) displays the heat maps' color scale with 1 representing high values and 0 representing low values. A comparison of Fig. 2(a) and Fig. 2(b) shows that there does not appear to be a visual correlation between the density of obese population locations and the number of high-calorie meals sold. This can be inspected by comparing the locations of the red areas between the two heat maps. The density of the high-calorie meals sold appears to be primarily centered within this simulation run, while the middle-right and middle-left positions within the environment contain a majority of the obese population. Additionally, the distribution of obesity appears to be largely stationed near the normal weight category (shown as white areas within Fig. 2(a)). This finding does not appear to directly support our hypothesis. However, there are several contributing factors that may influence this visualization, such as the fact that we created Fig. 2(a) using the home locations of the People agents, so a heat map of obesity distribution based on workplace location exclusively or a heat map based on an averaged obesity distribution based on home and workplace locations may provide better insight. After conducting and inspecting replications, our hypothesis does appear to hold.

For our second hypothesis, we expect eating habits to have a significant effect on the



(a) BMI density of population.

(b) Restaurant distribution.

Figure 3: Test case 2

level of obesity after 15 years. For this experiment, we assign a low-calorie eating habit to all people. We maintain the same set of outputs of interest and verification checks from the previous case. In addition, we also want to confirm that none of the meals came from the top 50% of calorie distributions from each restaurant. Fig. 3(a) displays a heat map of the density of obese people at the conclusion of the run while Fig. 3(b) displays a spatial plot of all of the restaurants' positions. An inspection of Fig. 3(a) quickly reveals that people are still able to become obese without eating high-calorie meals. Fig. 3(b) shows that the distribution of restaurant locations appears to more closely resemble a uniform distribution than the first test case. A larger sample size is required to make a final determination, but this is a promising outcome. A heat map of high-calorie meals sold during revealed that zero was produced which successfully passes the extra verification check for this test.

From the verification perspective, people with healthy eating habits becoming obese does not contradict any specific assumption from the model design and does not necessarily constitute an error. However, this raises several questions with respect to the model's validation and reveals that this is an area which requires further exploration. This could indicate that the minimum and maximum values of the restaurants' calorie ranges are too high or low, that the calorie range adjustment for each eating habit (i.e. top or bottom 50%) is too large, or that the BMR equations are not updating correctly within the agents.

Ultimately, this issue results from an oversimplification of the model's assumptions in that we do not account for physical activity. By incorporating the BMR equations without modifications based on the activity, we have unintentionally constrained the model so that nobody is physically active. With this constraint taken into account, Fig. 3(a) is a believable outcome for the model. However, to bring the model in line with hypothesis 2, the model will have to be adjusted to account for physical activity and its effect on BMR and V&V will need to be re-conducted.

5 Discussion

Creating the mentioned plots only require obtaining each agent's x and y coordinates, the initial values of parameters pertaining to the outputs of interest (e.g., eating habit), and the final values of parameters pertaining to the outputs of interest (e.g., weight). Our methodology includes a number of limitations under which its use may not be feasible. As reported by [6] and [36], visualizations become unwieldy for analysis when exploring dozens or more simulation runs at a time and that it is best suited for small sets of runs. While our use case focuses on the post-execution examination of single runs, heat maps can also be used at runtime to convey changes, illuminate clustering, or display variable distributions for the whole population. Additionally, these tests do not confirm that the model is completely error-free, they simply confirm that no errors were found with respect to the specific runs and output data involved with creating the spatial plots and heat maps. Additional tests are required for verifying assumptions or answering questions not directly associated with these tests.

A benefit provided by the use of heat maps is the ability to show the same data set under multiple perspectives, such as displaying the prominent areas of obesity along with the prominent locations of high-calorie meals sold. This allows for quick, informal comparisons to help determine if relationships appear to exist between agent types. Model constraints can be checked for violations or inconsistencies using visualization. In addition to heat maps and spatial plots, other visualizations, such as box plots and Q-Q plots, can further communicate differences between simulation results and the real system data for V&V [25].

As an initial V&V step in checking for unexpected behaviors, visualizations provide an intuitive interface for drawing inferences about the correctness of the simulation's execution and can help the modeler to select appropriate follow-on techniques. Our approach aids in the verification of some of the model's assumptions and constraints (those that pertain to the hypotheses being tested) while working to validate model hypotheses. Additional tests should still be conducted before formally accepting or rejecting hypotheses. The minimal background knowledge required to examine these graphics combined with the minimal data collection efforts needed from the simulation provides potential as a general approach for identifying unexpected behaviors within ABMs.

6 Conclusion and Future Work

We present an approach for identifying unexpected behaviors of ABMs that has the potential to enhance V&V practices for ABMs. We utilize a combination of spatial plots and heat maps to allow modelers to explore the interactions within their models. Heat maps allow for the creation of insight into the model based on visualization of the output data from the model. These explorations can assist the modeler in understanding how and why macro level behaviors are appearing within the simulation and guide the modeler in conducting additional tests. Spatial plots and heat maps are ideal for verifying and validating ABMs as they are suited for revealing the results of interactions between agents. We note that other types of visualization techniques can provide additional insights and can be further explored as future work in ABM V&V research.

Our use case conveys the ease of use involved with searching for unexpected behaviors of ABMs through visual inspection. Identifying assumptions, constraints, boundary conditions, and outputs of interest may be the most challenging aspect of our approach as it requires a high level of familiarity with the model. However, it does help to ease some of the knowledge requirements for V&V by removing the need to understand how to conduct statistical tests. The created visualizations assist in communicating how the model works, why certain outcomes occur, and increase confidence that the model's results are trustworthy. It remains the purview of the modeler to use proper visualization practices within these visualizations to convey the information in a manner that does not mislead its viewers. While we applied our approach to a snapshot of the simulation outcomes, these visualizations can also be applied during runtime to gain real-time insight into the dynamics of the agent behaviors.

Future work involves connecting our approach with existing V&V techniques to more efficiently explore the solution space and identify unexpected behaviors. This includes designing methods for automatically filtering the created spatial plots and heat maps to reduce the volume of graphs that need to be examined to only those containing potentially suspicious outcomes. For instance, [11] present an enhanced trace validation method for ABMs which facilitates SME insight without visualization by leveraging existing work in the field of statistical debugging. This method could be utilized in conjunction with visualization techniques to quickly isolate the causes of unexpected behaviors once identified. As a complementary approach to visualization, the use of sound can be explored as an option for revealing unexpected behaviors during runtime, such as ongoing work in [7]. Another avenue for future work includes an examination of what combinations of visualization techniques are best suited for identifying different classifications of unexpected behaviors, such as using heat maps to examine macro-level obesity behaviors while using Q-Q plots to compare distribution-based model assumptions against their actual distributions.

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