Microscopic Modeling Using a Discrete Element Method Clustering Technique
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ABSTRACT

This paper presents a dynamic intermodal freight network scheme using a Discrete Element Method (DEM) approach for performing the microscopic simulation. The model is applied to a roadway network for freight movements from a port terminal. This approach was used to develop efficient control strategies for optimizing freight flow. The simulation model has various applications with the primary focus the ability to access information about roadway conditions used by freight movements in real time. This paper describes the assumptions used to develop this model and the unique data flow scheme based on a micro-particle approach is presented. The performance of the simulation model is validated by comparing its performance with that of the Federal Highway Administration’s microscopic simulation model CORSIM.

Key Words
Traffic Simulation, Parallel Computation, Relaxation of Complex Systems, Shortest Paths, Discrete Element Method, Microscopic Transportation Modeling

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1.0 INTRODUCTION

Schemes which optimize transportation systems require tools that can integrate complex traffic networks and corridors. Also needed is the ability to capture data at any point and time within the network for the evaluation of the optimization scheme. One transportation network where optimization schemes are needed is on roadway networks used by freight transport. Trucks converging into a common port area for deliveries and shipments are one cause of major traffic congestion in our country. Without the ability to model these roadway networks, control strategies and optimization schemes have limited ability to improve traffic conditions. Microscopic simulation models describe the stochastic behavior of vehicles or objects in an integrated network. These models are less costly than field studies and are capable of estimating the impact of future traffic demands on roadway networks through the use of historical data.

In this paper, a conceptual freight simulation model is described. The model provides an approach to realistically consider variables related to intermodal freight movement. The freight movements considered in the simulation are freight movements from the terminal to adjacent roadway networks. The research focused on the dynamic effects of queue spillover, network traffic patterns, and performances of trucks picking up and delivering freight at the port terminals. The research also investigated the impact of these movements on entry/exit conditions at the terminal gate and the operation of signalized intersections within the port network. The model can also simulate a third dimension corresponding to grades in the alignment of the roadway. With this feature, the impact of grades on truck movements can be realistically simulated in the model. The paper describes the data structure and the conceptual model is discussed in detail. The parallel application and the three dimensional model is not discussed in this paper, but will be included in a subsequent paper.

2.0 BACKGROUND

Many micro-simulation models have been developed for various traffic networks. The simulation model developed in this research uses a Discrete Element Method (DEM). This method was employed as it can be integrated with other applications, and can be used both for high density systems and on a macro-scale. In a high-density system, vehicle–vehicle interactions are based on car-following theory. In a macro-scale, cars within the links of the network behave as an ideal gas as assumed in some traffic theory models. No unified theory has been developed for describing all traffic flow conditions. This approach allows the following to occur:

1) To explore technological innovation prior to traffic field studies;
2) To perform rigorous parametric studies; and
3) To examine data that is normally inaccessible.
The discrete element clustering technique can be used to:

1) Directly relate the macroscopic performance of traffic flow to intrinsic properties that define vehicle operation;

2) Develop new continuum models that link the information at the micro, meso and macro scales; and

3) Provide detailed information about what happens within the vehicle systems and thereby provide a rational framework for decision making with regards to route guidance.

The discrete element method approach also has the advantage of having the potential to be scaled up to a large scale parallel computing model. Previous research has been performed on the use of large scale parallel computing for traffic modeling. Dynamic assignment models have been developed using this approach. Ran and Shimazaki (1989) proposed dynamic user optimal traffic assignment models that consider departure time choice, route choice, and stochastic route travel times. Junchaya (1992) demonstrated that a parallel machine can handle a much larger network capacity. In that work, parallel computing was used to simulate a 32,000 vehicle network using a predetermined path for all of the vehicles. Junchaya used parallel computing architectures to simulate a large-scale traffic network with sufficiently fast response time for real-time operation. The methodology to simulate a traffic network was described for a Connection Machine, CM-2, a massively parallel computer. This Connection Machine architecture was equipped with 16,384 processors. This research expanded this idea to allow for vehicles to be guided by a Origin and Destination (O-D) coordinate system, giving individual vehicles the ability to change lanes and make turns as needed.

Nagel (1994) presented a simple rule-based approach for developing a microscopic simulation model. In this case the size of the network was measured by lanes or kilometers. The parallel computers, Parsytec GCel-3, Intel iPSC/860 and the Connection Machine CM-5 were employed as the computer architecture. Also a comparison was made between NEC-SX3/11 single node vector computer and a net of coupled workstations. A 1000 times faster performance was noted when compared to published computing speeds of microscopic traffic models. The simulation model was limited to a one-dimensional problem. In the research the particle-oriented approach was abandoned because of the problem with distributed memory arrangement in multi-lane traffic. It was noted that the computational demands becomes costly and complicated because of dynamic memory assignments.

Nagel and Rickert (2001) in a more recent work at Los Alamos developed a parallel computing approach using a microscopic technique called Cellular Automata (CA). The parallel algorithm incorporating this technique is called, TRANSIMS, and it incorporates a route planner, microscopic traffic simulation, along with an iterative re-planning for dynamic route assignments. In the research performance figures were presented for street networks with up to 20,000 links.
Papageorgiou (1998) mentioned that many have argued that macroscopic traffic models lack the descriptive accuracy level that are achieved in other disciplines. However, the discrete element model is a microscopic model that has been successfully developed for interdisciplinary purposes. As most of the simulation models described above, the discrete element model in this research has parallel capability for analyzing traffic patterns, link travel time optimization, and network performance. The interdisciplinary nature of the model allows the model to be applied to other modes of transport, for example for traveling on mountainous terrains (3-D). The validity of the discrete element model approach and its performance for the discipline of freight modeling is presented in this paper.

3.0 DEM CLUSTERING APPLICATION

Numerous micro-mechanical models based on DEM have been used to study the micro-mechanics of particles. In brief, DEM is a method that can model an assembly of particles on an elemental (discrete) basis. The technique was founded by Cundall and Strack (1978, 1979), who employed this technique to describe the behavior of rocks collapsing under the load of gravity (Cundall, 1971). Since then, DEM has been widely adopted in powder and grain technology and soil mechanics.

To apply DEM to traffic modeling, the following assumptions were made:

1) Prevailing speeds and vehicle motion were based on gravity effects as found in Cundall’s model; and

2) Boundary walls, defining the limits of the roadway network to be simulated, were assumed stationary and vehicles entering/exiting the network were based on these boundaries.

The application of a discrete element model that remained consistent in the traffic model were:

1) All vehicles in the system could be motioned independently based on their current speeds;

2) Each vehicle had to be tracked and boxed within a spatial area and memory location;

3) Contact detection was performed to prevent overlapping of vehicles in the network; and

4) Constitutive Laws (in this case a car-following theory) described the effects of the nearest neighbor ahead of it.

In the past, other researchers have used Discrete Element Method to simulate dynamic behavior. One of the advantages of using this approach is that models based on DEM consider the behavior of individual particles and can handle discontinuities such as queues and spillovers in the network. Since, the driving force of this traffic model for each vehicle are prevailing speeds and velocities, global network behavior is determined through a series of calculations that trace the movements of individual particles or vehicles.
The DEM model developed in the research was designed to handle a large number of vehicles. As a result, the clustering of these vehicles became necessary for scalability and for adaptation to a parallel machine. A cluster was considered to be one intersection and its adjoining links as shown in Figure 1. Clustering in a network is an essential feature of the algorithm, since multiple processors can be assigned to groups of vehicles as opposed to analyzing one vehicle at a time.

**4.0 DYNAMIC ACQUISITION TRANSPORT OPTIMIZATION (DATO)**

The algorithm developed incorporating the constitutive laws describing the car-following behavior is named Dynamic Acquisition Transport Optimization (DATO). DATO follows the steps of a parallel computing DEM algorithm, but it incorporates a clustering technique. DATO is a modification of an algorithm, Trubal for Parallel Machine (TPM), where TPM is a parallel computing simulation model based on Discrete Element Method. The data structure of TPM numerically models a dry granular material by using an explicit finite difference formulation. TPM was developed to simulate the micro-particle behavior for assembly of dry granular particles (Washington, 1996). The simulation was developed on massively parallel supercomputers (CM-5 & CM-2) by implementing a data parallel structure. In the model, a network of linear springs connects particle-shaped masses to describe the contact laws. The TPM data structure for mapping particles for contact detection is shown in Figure 2 to explain the origin of DATO’s traffic models scheme, and its adaptation of a clustering technique. The figure shows the layout of particles that are placed strategically in a memory location within computer’s architecture when arrays are initialized, so that a particle’s nearest neighbor will be within the same processor’s memory allocation or the neighboring processor. This allows for low computer latency and a better performance in retrieving parameters for calculations between neighboring particles. The figure graphically depicts a three dimensional array and the particles are shown boxed within the spatial grid of this memory allocation.

TPM was initially designed for a Single Instruction Multiple Data (SIMD) platform, based on its inherent data parallel platform. This means that for each line of instruction multiple data can be generated from each processor to execute various calculations within the matrices. Washington (1996) discusses the TPM mapping of matrices for particles on an SIMD platform in detail.

The DATO simulation model exploits high performance computing and imitates the response behavior expected from individual vehicles found on the freight transportation road systems in Port Elizabeth and Newark in New Jersey. Similar to other traffic models which view traffic flow as an ideal gas or compressible fluid, the discrete element model views traffic flow as an assembly of independent particles which behaves as a continuum with boundary conditions (entry/exits gates) but also can allow for non-linear interaction and discontinuities between neighboring particles. Each vehicle is encompassed by a disc which defines the space occupied by the vehicle and additional space or tolerance to prevent the vehicle from a virtual collision with another neighboring vehicle. The tolerance within the disc is used as a mechanism that enables the vehicle’s speed to be adjusted when the disc overlap with other vehicle discs that may be following, leading, or changing lanes within the link.
The DATO program simulates a two or three dimensional model with periodic boundaries. For this model of the intermodal freight movement, the periodic boundaries are taken to be at the terminal exit/entry gates. The periodic effect is allows one vehicle to leave the network, and reenter at a different time into another entry, mimicking the effects of a larger network. The entrance and exits of vehicles into the system also changes the speeds achieved by vehicles, as these entries affect link concentrations and densities. The assumptions is that as vehicles are added or removed from the links, the concentrations will increase and decrease respectively, causing the car following laws to regulate the speeds accordingly. Variable densities within the links is also due to the effects of the origins and destinations of vehicles within the links. The amount of vehicles with short travel paths will be affected mostly by the periodic boundaries because as they exit they re-enter at another location at designated times. This operation simulates the effects of a small network within a much larger network.

5.0 DATO ALGORITHM

Subroutines used in the DATO algorithm subroutines are generalized in the flow chart provided in Figure 3. The six primary routines that govern the performance of vehicles in the simulation are the SETUP & INITIALIZE routines, the CYCLE routine, the MOTION routine, the VEHICLE routine, the CONTACT routine, and the IMAGE AND OUTPUT routine.

The SETUP & INITIALIZE routines initialize all variables for the algorithm and also map vehicle information into specified memory location on the architecture. It adds vehicles to the system at a predetermined schedule imitating trucks arriving and departing at the terminal gates. The routine also assigns vehicles to the roadway network using either a predetermined or random path. Parameters specific to particular vehicle types used in the model are created based on input variables. Some of these parameters include vehicle mass and size.

In the CYCLE routine, the time interval is set for each time step and the number of time steps required to complete the entire simulation are set. The remaining subroutines are called including routines that update vehicle position, control the signalized intersections, and the entry/exit of vehicles in the network. The time-steps or cycles will terminate once all of the equipped vehicles with preset origin and destination routes have completed their travel time. Hence, the performance of the network can be measured by the duration of the simulation model.

In the MOTION routine, vehicles are motioned based on the prevailing speeds and concentration within the link. Initially, there are no vehicles within close proximity of each other so they are motioned based on the prevailing speed that is preset for each link. The default prevailing link speed reduces with increasing traffic volumes. When the link resumes a lower volume, vehicle speeds decrease to default speed values. Leading vehicles and traffic signals are the only other controls on vehicle speeds. The advantage of DATO’s data structure over TPM’s data structure is that the updated vehicle speed and distance is only dependent upon leading vehicles and traffic signals in its local link, and not a 3-dimensional summation of all its neighboring particles as in TPM. This relatively smaller particle interdependency produces less communication latency and increases the performance of a parallel computing systems.
The main governing equations used to determine vehicle speeds within the network is expressed by the relationship:

$$ma + cv + \beta x = F(t)$$  \hspace{1cm} (1)

where $m$ and $c$ are respectively the vehicle’s mass and damping, and $\beta$ has been modified to represent the car-following interaction coefficient for two vehicles with overlapping tolerances, and $a$, $v$, and $x$ are the vehicles’ acceleration, velocity, and distances of overlapping disc (vehicles) respectively. The first part of the equation is represented by Newton’s Second Law which can be written as follows:

$$m_i(a_{i,x,y}) = (F_{i,x,y})_N$$  \hspace{1cm} (2)

where “$i$” designates the number assigned to the vehicle and “$x$ and $y$” are the components in two dimensions as shown in figure 4. In this expression the $F_i$ is the net force at the beginning of the time-step, $t_N$. The finite difference scheme, used to integrate the system’s equations of motion, uses the subscript $N$ to represent the beginning of the current time step, and $N-1/2$ or $N+1/2$ for denoting the new result for the current time step. Since the accelerations $a_i$ are constant over the interval $t_{N-1/2}$ to $t_{N+1/2}$, then the vehicle velocities can be calculated as:

$$v_{i,N+1/2} = v_{i,N-1/2} + [(F_{i})_N \Delta t / m]$$  \hspace{1cm} (3)

This relationship is used to describe vehicle velocities for all vehicles that are traveling less than the prevailing speeds for that link. In this equation the final velocity at the end of the time-step is determined by the initial velocity plus whatever speed reduction or increase is calculated based on the acceleration or deceleration of the leading vehicle. This behavior is described as $F$, the force due to a leading vehicle. The force is defined in equation 3 as a function of vehicle interaction within the link. Other velocity controls are due to the prevailing speeds which vary as the concentration in the link changes and as vehicles approach a changing traffic signal.

The VEHICLE routine is responsible for automating the destination of vehicles. This destination is random and is controlled within the intersection by determining whether the vehicle makes a left, through or right-turn (see Figure 5). Figure 5 shows that each box within the intersection is designated for vehicles that are traveling in a particular direction. Vehicles approaching a given box (shown as clear circles) make turns based on preset percentages (shown as cross hatched circles). This feature allows for a larger network of vehicles to be simulated as each vehicle no longer requires a specific traffic assignment pattern. This feature is similar to CORSIM’s modeling approach which also uses preset percentages for determining the number of vehicles turning at an intersection. Speed reduction is also controlled within this turning activity and turns are blocked when other vehicles prevent turning movements from occurring.

In the CONTACT routine the Force, which represents the leading vehicle, is directly proportional to the velocity since acceleration is constant for each time step and produced by vehicle interaction. The car-following mechanism is based upon the amount of overlap found between two discs (see Figure 4). Since the vehicles are encompassed by a disc with a specified tolerance, the overlap does not imply collision but is used as a mechanism for achieving a reduction in speed or deceleration. For example, each disc (vehicle) checks for potential
overlaps with a disc in front of it for other neighboring vehicles. If a disc (vehicle) is found to have an overlap, then a negative force (or velocity) is produced to slow the vehicle down proportional to its overlapping distance. The contact forces are calculated using an incremental force-displacement law of the form:

\[ (F_n)_{N+1} = (F_n)_N + (\Delta F_n)_N = (F_n)_N + \beta_{N+1/2} \]  

where \( F_n \) are the normal forces, and \( \beta_n \) has been modified to represent the car-following interaction coefficient for two vehicles with overlapping tolerances (see Figure 5). The overlap of discs is represented by \( \Delta_n \) and can be written as:

\[ (\Delta_n)_{N+1/2} = [(d_{b_i} - d_{a_i})]_{N+1/2} e_j \Delta t \quad i = x, y \quad j = 1 \ldots \# \text{ of links} \]  

where \( (d_{b_i} - d_{a_i}) \) is the relative distance between two overlapping discs (vehicles) \( a \) and \( b \), and \( e_j \) is written as:

\[ e_j = \frac{v_j}{l_j} (j = 1 \ldots \# \text{ of links}) \]  

where \( v_j \) is a speed function preset for each link and \( l_j \) is the length of each link. Vehicles resume prevailing speeds, which are subject to link concentrations, when the contact is broken. Lane changing is also affected in this routine. If a vehicle is traveling in the \( x \)-direction and an overlap distance is detected in the \( y \)-direction, it will not be permitted to change lanes, and its speed will not be affected.

The **IMAGE AND OUTPUT** routine creates a snapshot of the roadway network in Portable Document Format (pdf) showing vehicle behavior at one time-step in the model. The routine also determines performance measures used to evaluate the performance of the roadway network. Some of these parameters include: the concentration of vehicles on each link; and the updated prevailing speeds for vehicles in the network, which are based on link concentrations. Output data regarding signalized intersections and route travel times for each vehicle is also retrieved for the control strategy or optimization scheme being tested. When the freight network system has reached an optimal flow for a given signal timing, that is, no queues exists at the intersections, the control strategy is deemed as working optimally.

### 6.0 SIMULATION RESULTS

Port Newark in Newark, New Jersey was selected as the port roadway on which to test the simulation model. Figure 6 shows a map of the port roadways indicating the roadway network used for modeling. For this simulation, roadways within the network were known to have vehicle queues at both signalized intersections and at entrances to terminals. Due to terminal schedules, an example of trucks blocking lanes is shown in Figure 7. The modeling of this condition is hampered by various factors. Some of the factors include:

1) Terminal schedules are unknown and vary with time and demands;

2) Drivers do not necessarily have on-board information about the time of their pickups;
3) Origin-Destination patterns are not known, therefore traffic control devices cannot be controlled to handle existing roadway patterns; and

4) The geometry of the streets is not detailed for imaging accurate travel distances from all sources.

As a result, a number of simplifications and assumptions had to be incorporated into the model in order to simulate this behavior. All roadways in the port area were modeled as straight links (see Figure 6). The contours of this network were relatively flat so that the third dimension (mountainous terrain) of this model was not used. Link lengths were approximated so that similar link lengths could be used in the validation model CORSIM.

The DATO files describing the intersections and links are seen in Figure 8. The traffic volumes used for this model were obtained from the Port Authority of New York and New Jersey, who operate Port Newark. Preliminary results from the simulation model are shown in Figure 9. The figure provides an image of vehicle queues in the network using a pdf file. Similar results using CORSIM are also provided in Figure 10.

The advantage of this discrete element microscopic model is: 1) its ability to acquire real-time information for optimal control strategies; 2) its application to a parallel architecture for scalability, and 3) its eventual ability to incorporate real-time communication technologies from various databases or information systems for simulated optimization. The darker particles in Figure 10 are vehicles which are tracked by the algorithm which enables those vehicles to receive dynamic on-board information at scheduling time (time step) or travel plan.

7.0 FUTURE WORK

The model and its results are in a data parallel structure which is applicable to the Single Instruction Multiple Data (SIMD) platform. The next phase of this research, is to port this code to the massively parallel computer, the Origin 2000, as other parametric studies are being performed. In addition, a Multiple Instruction Multiple Data (MIMD) platform is currently being tested involving high performance PCs clustered together using a Parallel Virtual Machine (PVM) software. This paradigm models an intermodal freight system for an integrated network by dividing the network geometrically amongst multiple processors. This approach allows contact detection to occur within local processors. In this case, the clusters described in this paper or multiple links/intersections are geometrically located in proximity to the same processor, because the interdependency of vehicles is localized at each link. As a result, the calculations are streamlined within the local memory of that processor allowing for message passing to be enabled when vehicles data are transferred to its neighboring processor. The integration process of the discrete tools is under development and will covered in subsequent papers.
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Figure 1. Clustering Scheme in DATO Algorithm
Figure 2. Trubal for Parallel Machine (TPM) Spatial Memory Allocation
SETUP & INITIALIZE
All parameters (i.e. velocity, signals, veh. contacts, destinations, etc) are initialized.

CYCLE ROUTINE
All routines are called (i.e. intersection, motion, contact, aplot). The max # of time steps and vehicles are set.

MOTION ROUTINE
Initially checks whether O-D vehicles have reached their destination. Finds vehicles in each link/intersection.

Does Vehicle have a Random Destination??

Vehicle Routine
All cars are turned in the intersection based on percentages/signals.

All cars make turns at the intersection based on destination coordinates/signal lights.

CONTACT ROUTINE
Checks vehicles in contact and adjust speeds of vehicles.

IMAGE AND PLOT ROUTINE
Draws the location of vehicles in network or prints network results (i.e. densities, volumes, etc.).

END SIMULATION

Figure 3. DATO’s Flow Chart
Figure 4. Vehicle Disc

Figure 5. Vehicle Intersection Boxes
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