Monte Carlo
A general overview of methods, theory and practice

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Lectures

- Lecture 1- Background and theoretical/analytical development of the Monte Carlo method
- Lecture 2- Numerical simulation practices and common techniques used in modern modeling applications
- **Lecture 3- A research project perspective: application to traffic flow**

Outline

- The traffic model: properties and dynamics
- Calibration and parameter estimation
- Simulations and comparisons (one-lane highway)
- Deterministic closures and macroscopic models
- Multi-lane extensions
- Conclusions & References

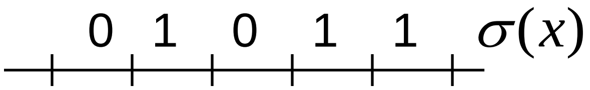
Proposed Traffic Model Properties/Attributes

- Asymmetric Simple Exclusion Process (ASEP)
- Arrhenius microscopic stochastic dynamics
- One directional flow
- Look-ahead interaction potential
- Retarded acceleration
- Timely braking
- Conservation of vehicles (assuming no entrances or exits)
- Numerical simulations via Kinetic Monte Carlo (KMC)
- Extensions to macroscopic traffic flow models and PDEs

Main Statistical Mechanics Concepts

We let Λ denote a lattice of N cells.

We also denote by $\sigma(x)$ the spin configuration at x.



We introduce the microscopic stochastic Ising process $\{\sigma_t\}_{t\geq 0}$

A spin configuration σ is an element of the configuration space $\Sigma = \{0,1\}^{\Lambda}$ and we write

$$\sigma = \{\sigma(x) : x \in \Lambda\}$$

The stochastic process $\{\sigma_t\}_{t\geq 0}$ is a continuous time jump Markov process on $L^{\infty}(\Sigma, R)$ with generator

$$Mf(\sigma) = \sum_{\substack{x\in\Lambda \\ y\neq x}} c(\sigma)[f(\sigma^{*}) - f(\sigma)]$$

The corresponding energy Hamiltonian is

$$H(\sigma) = \frac{1}{2}\sum_{x\in\Lambda} U(x)\sigma(x)$$

where the interaction potential is given by

$$U(x) = \sum_{\substack{z\neq x \\ z\in\Lambda}} J(x,z)\sigma(z) - h$$

where J denotes the local interaction potential

$$J(x,y) = \gamma V(\gamma\,|\,x-y\,|)$$

Here $\gamma = 1/(2L+1)$ and L denotes the interaction radius.

Equilibrium states of the stochastic model are described by the Gibbs measure $\mu_{\beta,N}$ at the prescribed temperature T,

$$\mu_{\beta,N}(d\sigma) = \frac{1}{Z} e^{-\beta H(\sigma)} P_N(d\sigma)$$

where $\beta = \frac{1}{kT}$ and $P_N(d\sigma) = \prod_{x \in \Lambda} \rho(d\sigma(x))$

and $\rho(\sigma(x) = 0) = \frac{1}{2}, \qquad \rho(\sigma(x) = 1) = \frac{1}{2}$

The Mathematical Model

$$\frac{d}{dx} Ef(\sigma) = EMf(\sigma)$$

where $Mf(\sigma) = \sum_{x \in \Lambda} c(\sigma)[f(\sigma^*) - f(\sigma)]$

and σ^* denotes a new lattice configuration

Microscopic Arrhenius
Spin-Exchange Dynamics

The Arrhenius spin-exchange rate c(x,y,σ)

$$c(x,y,\sigma)=\begin{cases} c_d e^{-U(x)}, \text{ if } \sigma(x)=1, \text{and } \sigma(y)=0, \\ c_d \mathrm{e}^{\text{-U(y)}}, \text{ if } \sigma(x)=0, \text{and } \sigma(y)=1, \\ 0 \qquad, \text{ otherwise} \end{cases}$$

With exchange rate constant, $c_d = \dfrac{1}{\tau_0}$

Here τ_0 denotes the characteristic time of the stochastic process.

Again recall that $U(x) = \sum_{\substack{z \neq x \\ z \in \Lambda}} J(x,z)\sigma(z)$

The Arrhenius spin-flip rate c(x,σ) at lattice site x and spin configuration σ is given by

$$c(x,\sigma) = \begin{cases} c_d e^{-U(x)}, & \text{when } \sigma(x) = 0 \\ c_a, & \text{when } \sigma(x) = 1 \end{cases}$$

With adsorption/desorption constants, $c_a = c_d = \dfrac{1}{\tau_I}$

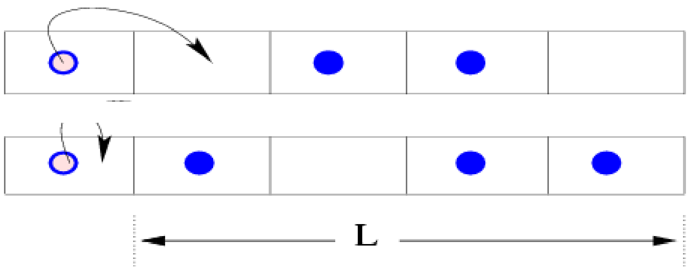
Here τ_I denotes the characteristic time of the stochastic process.

We consider short vehicle potential interactions J,

$$J(x,y) = V(\gamma(x-y)), \qquad x,y \in \Lambda$$

where $\gamma = 1/L$ as usual ordains the range of microscopic Interactions.
Here $V : R \to R$ via,

$$V(r) = \begin{cases} J_0, & \text{if } 0 < r < 1 \\ 0, & \text{otherwise} \end{cases}$$



Which enforces:

- Exclusion princile
- Vehicles do not go backward in traffic
- Local effect of the interactions

(thus once again, more realistic traffic conditions)

The Traffic Model

$$\frac{d}{dt} Ef(\sigma) = EMf(\sigma)$$

or in more detail,

$$\frac{d}{dt} Ef(\sigma) = E \sum_{\substack{x \in \Lambda \\ y \neq x}} c(x, y, \sigma)[f(\sigma^*) - f(\sigma)]$$

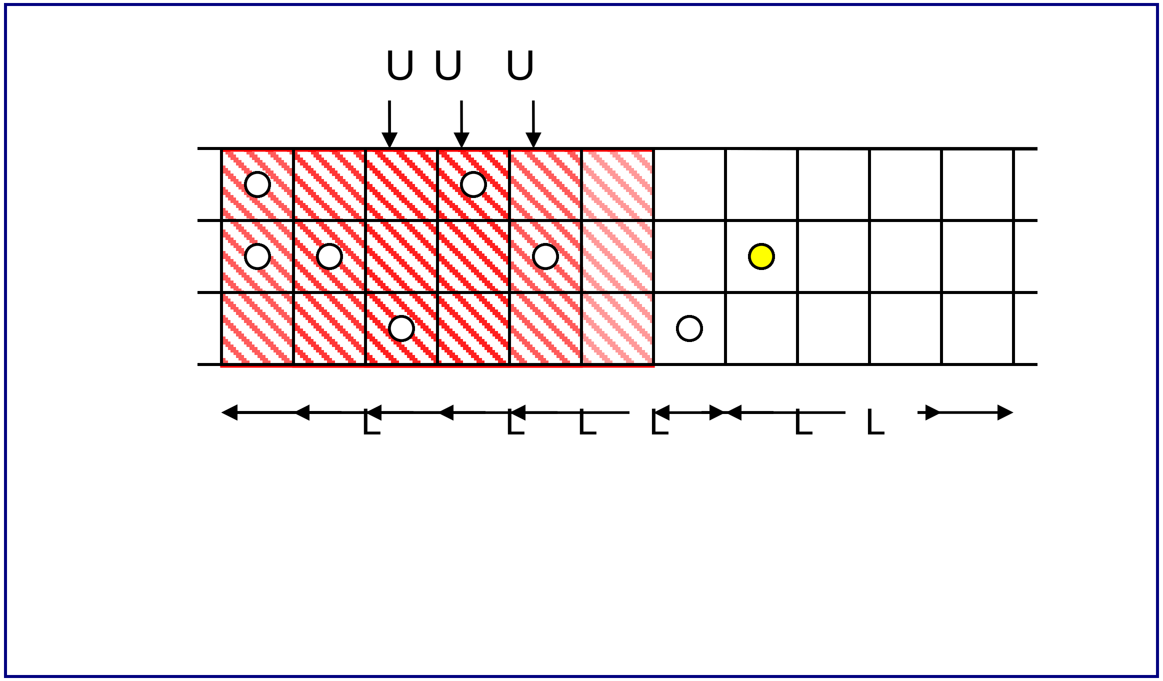
which based on the spin-exchange rate c(x,y,σ) for y=x+1 gives,

$$\frac{d}{dt} Ef(\sigma) = E \sum_{x \in \Lambda} c_0 \sigma(x)(1 - \sigma(x+1)) e^{-U(x,\sigma)} [f(\sigma^{x,x+1}) - f(\sigma)]$$

The probability of a spin-exchange between x and y=x+1 during time [t, t+Dt] is

$$c(x, y, \sigma)\Delta t + O(\Delta t^2)$$

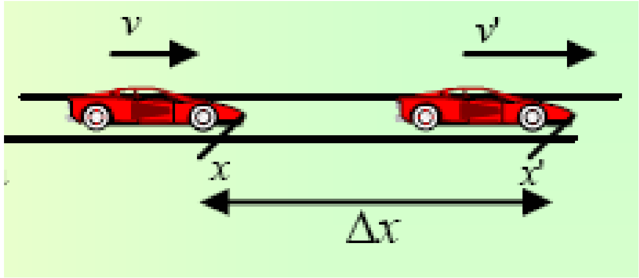
A simple schematic describing the traffic model dynamics



Free Parameters and Calibration

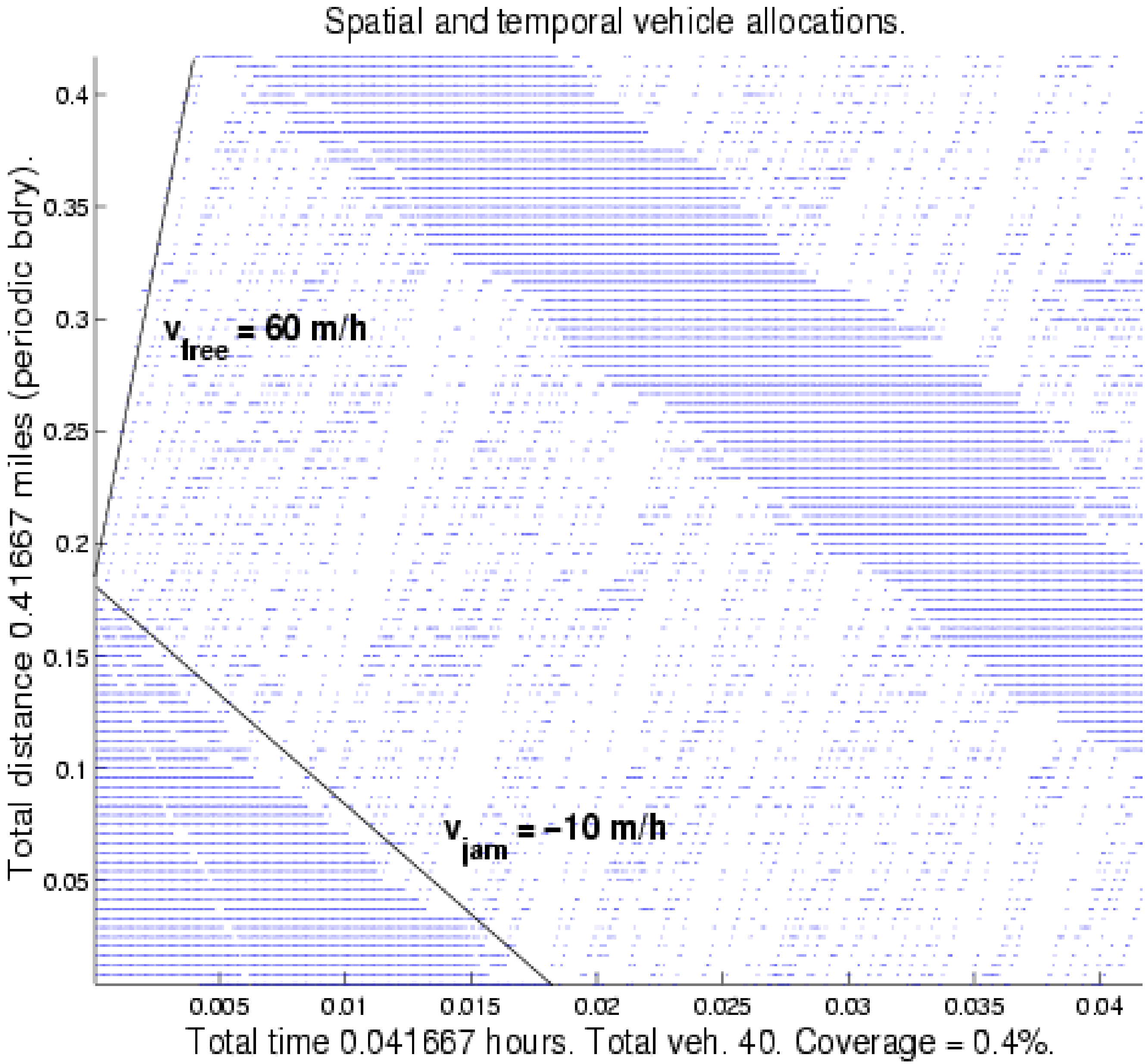
The model is characterized by the following three undetermined parameters:

- τ_0 - the characteristic time of the stochastic process
- J_0 - the strength of the interactions
- L - the interaction potential range

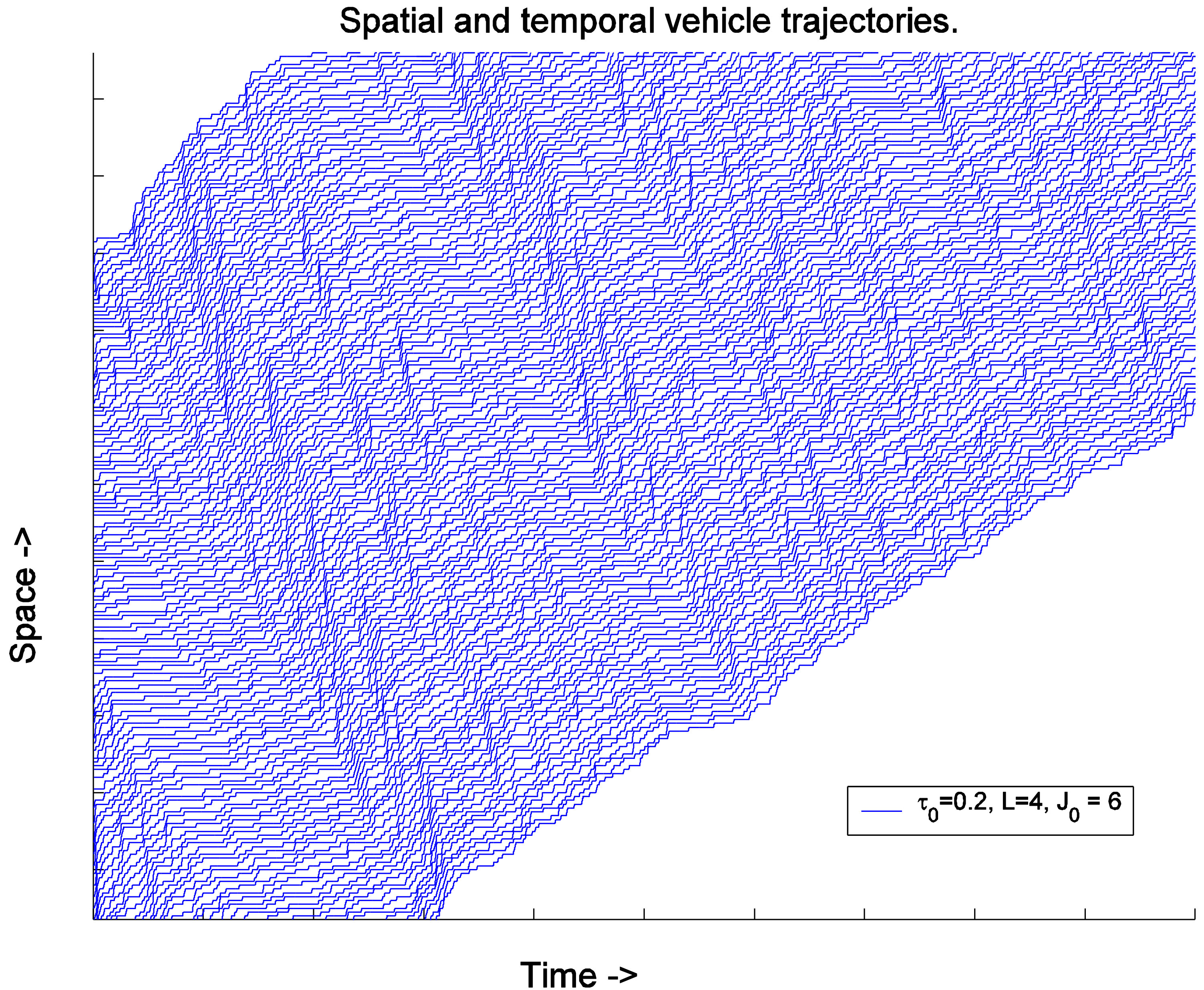


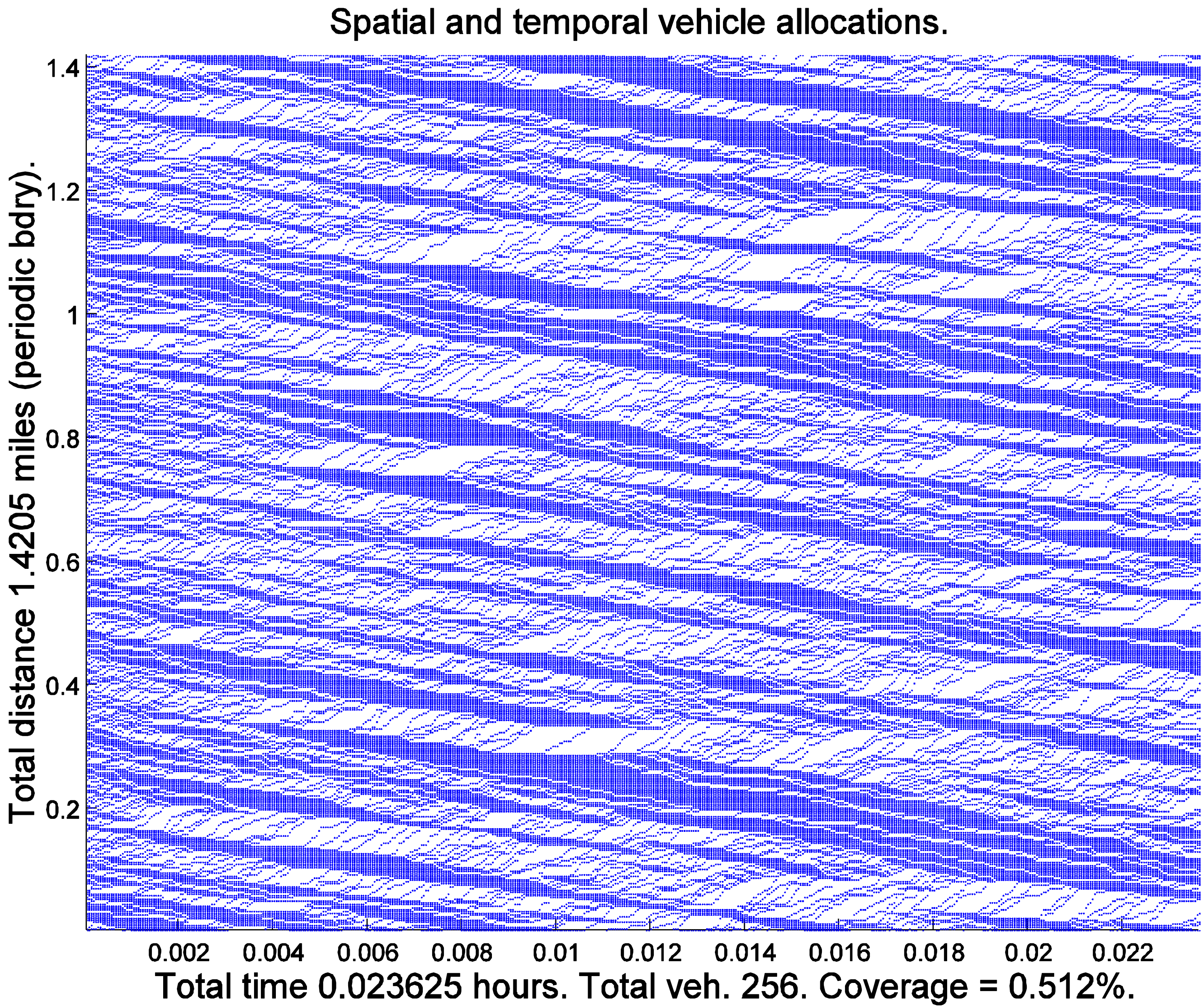
Cell length is assumed to be 22 feet (average vehicle size plus safe distance).

$$\Delta t_{cell} = \frac{22\,\text{feet}}{65\,\text{miles/hour}} \approx \frac{1}{4}\,\text{sec.}$$

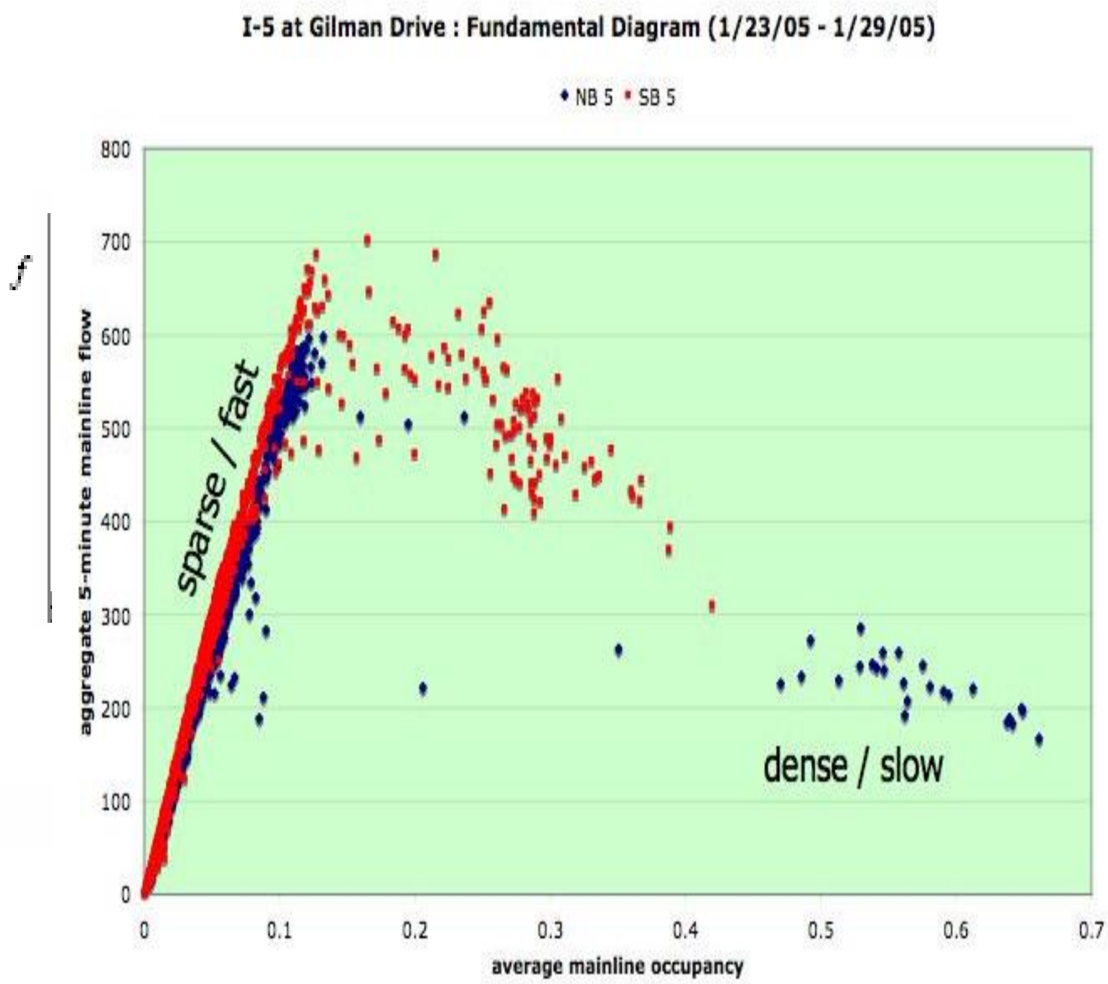


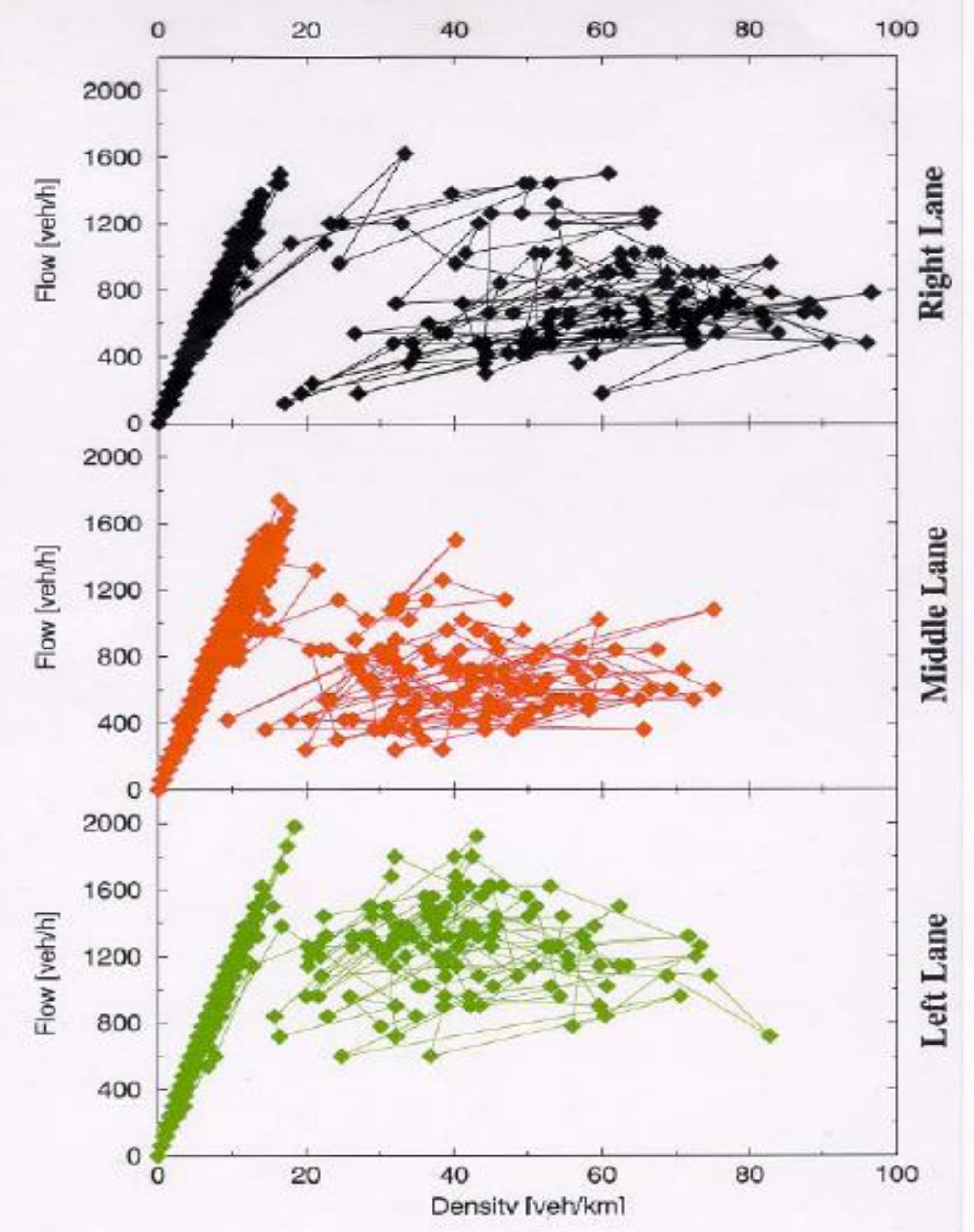
Spatial and temporal vehicle allocations.
v_{free} = 60 m/h
v_{jam} = −10 m/h
Total distance 0.41667 miles (periodic bdry).
Total time 0.041667 hours. Total veh. 40. Coverage = 0.4%.
0.4
0.35
0.3
0.25
0.2
0.15
0.1
0.05
0.005
0.01
0.015
0.02
0.025
0.03
0.035
0.04


Spatial and temporal vehicle trajectories.
Space ->
Time ->
τ_0=0.2, L=4, J_0 = 6

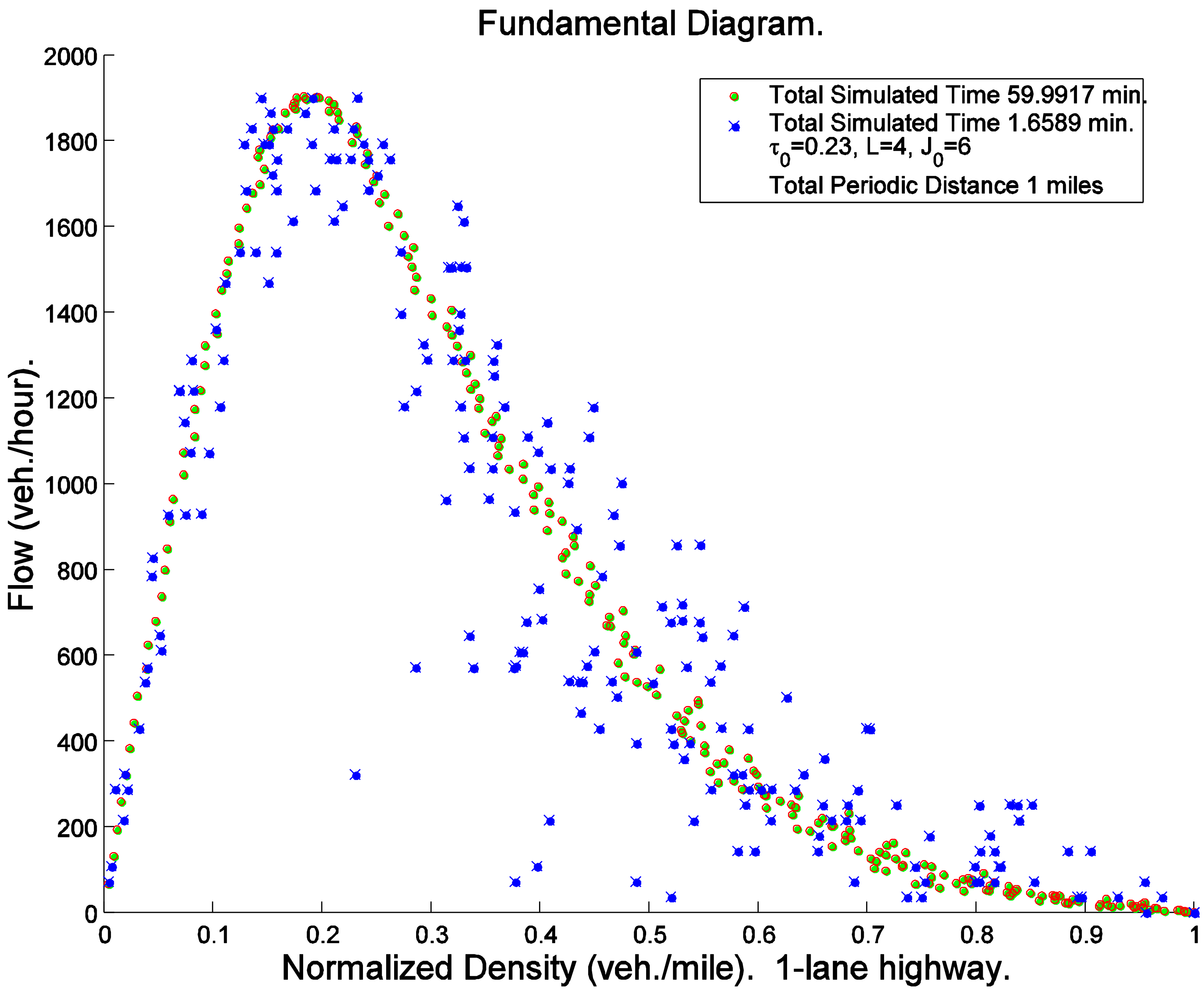

Spatial and temporal vehicle allocations.
Total distance 1.4205 miles (periodic bdry).
0.2
0.4
0.6
0.8
1
1.2
1.4
0.002
0.004
0.006
0.008
0.01
0.012
0.014
0.016
0.018
0.02
0.022
Total time 0.023625 hours. Total veh. 256. Coverage = 0.512%.

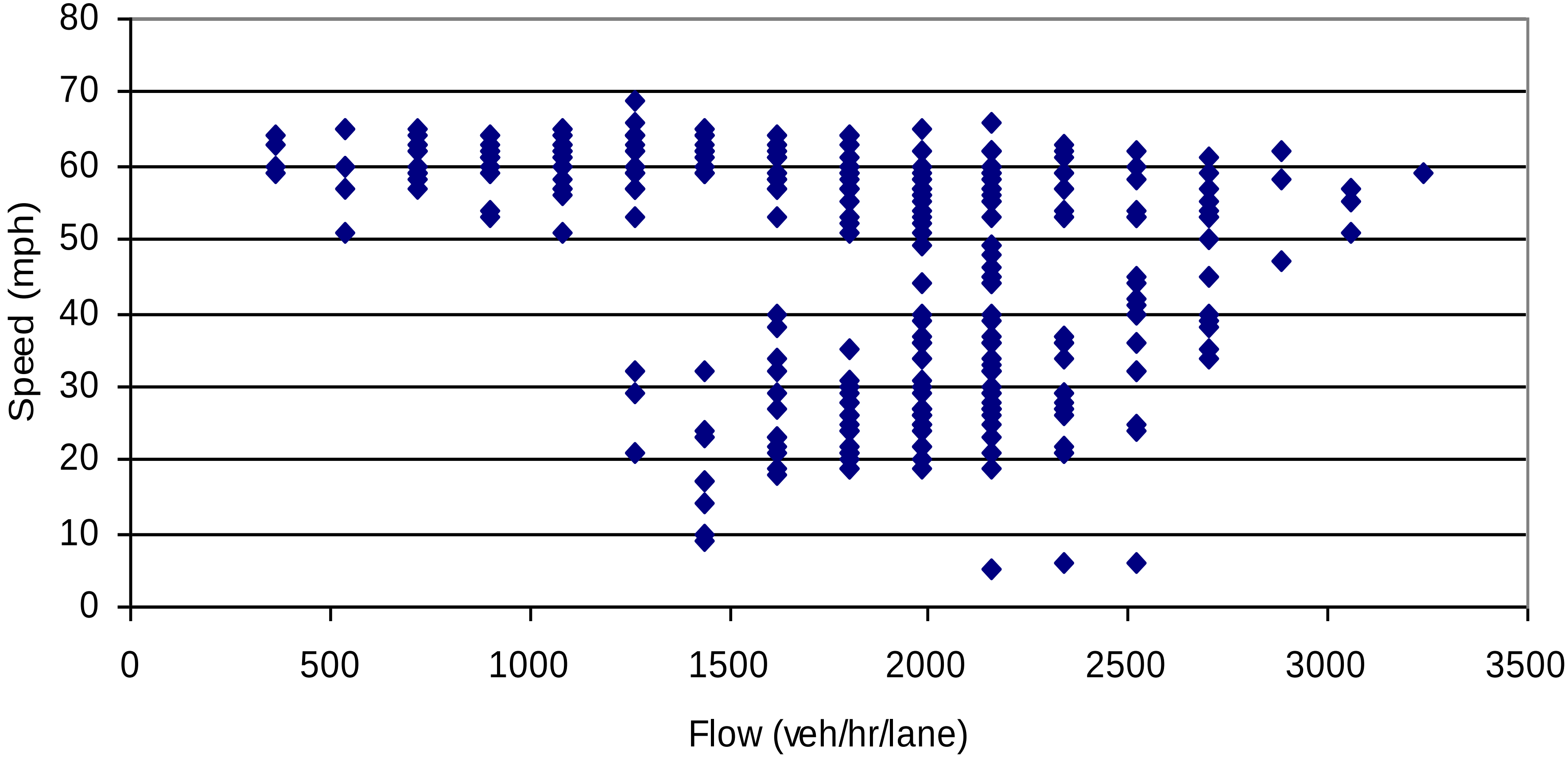
Flow-Density Diagram
Experimental Data



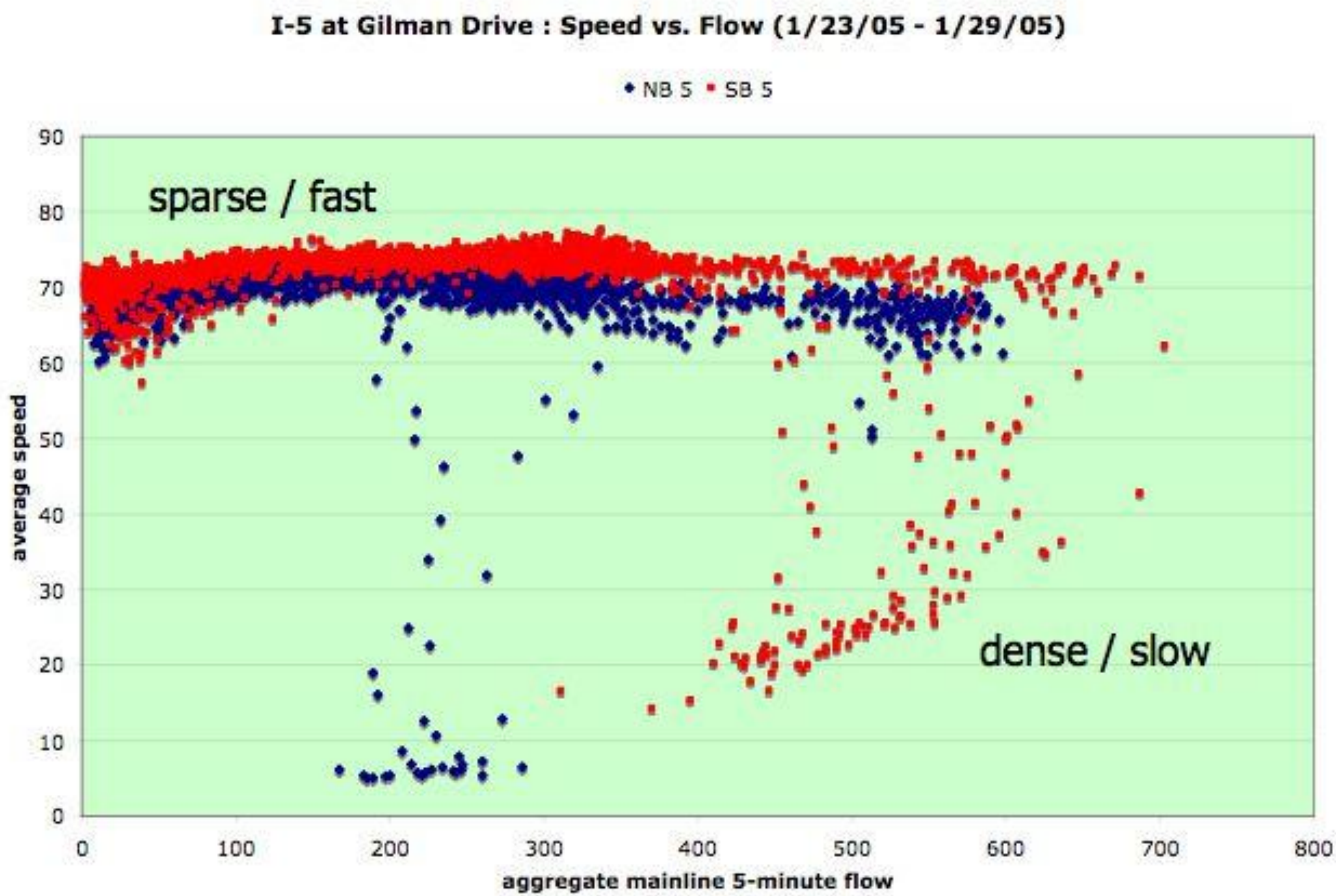


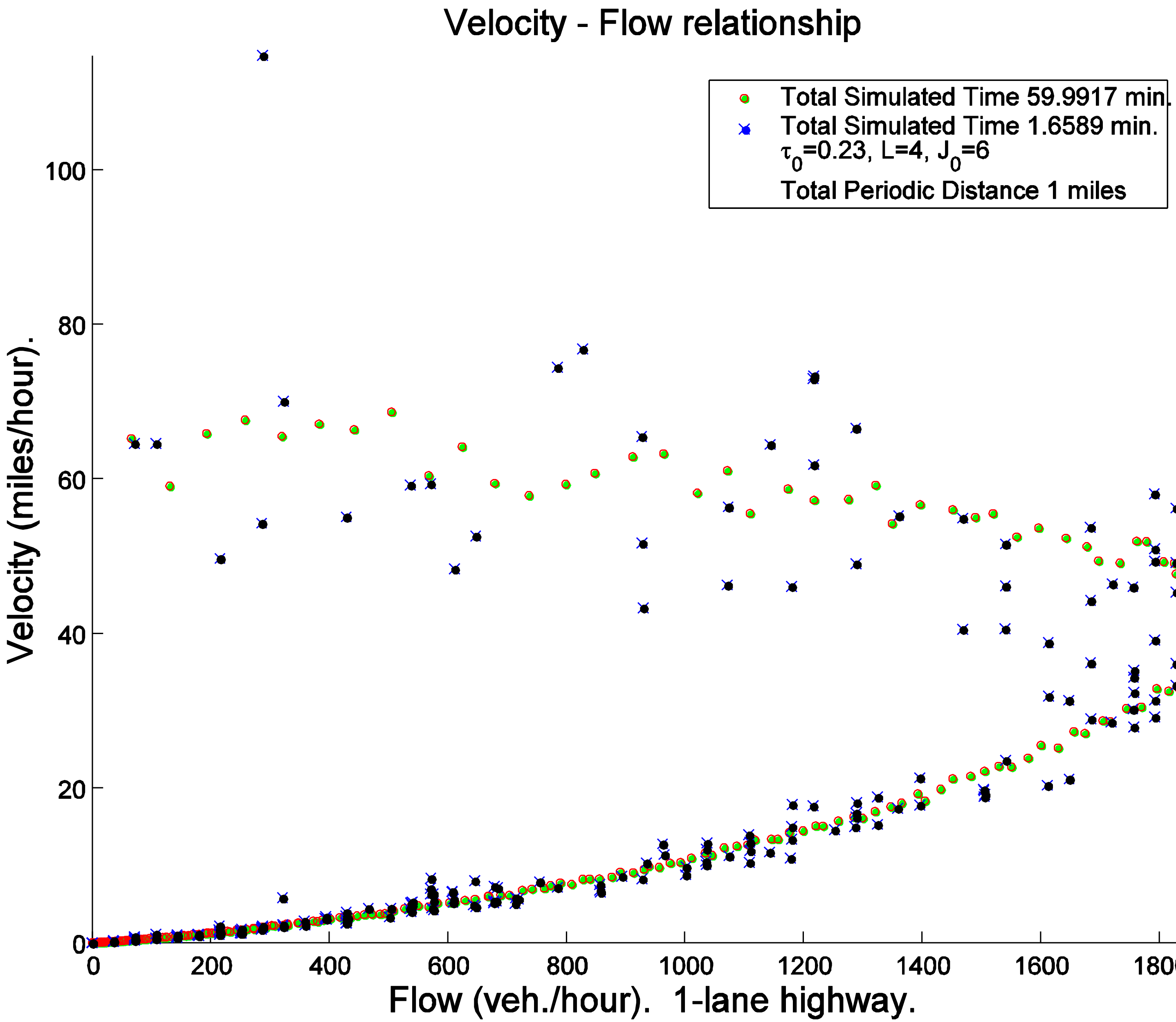
0
20
40
60
80
100
2000
1600
1200
800
400
0
Flow [veh/h]
Right Lane
Middle Lane
Left Lane
Density [veh/km]


Fundamental Diagram.
Total Simulated Time 59.9917 min.
Total Simulated Time 1.6589 min.
τ_0=0.23, L=4, J_0=6
Total Periodic Distance 1 miles
Flow (veh./hour).
Normalized Density (veh./mile). 1-lane highway.
0
200
400
600
800
1000
1200
1400
1600
1800
2000
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1



Velocity-Flow Diagram (real freeway data from San Antonio) [Halkias & Mahmassani (MTI 2005)]


I-5 at Gilman Drive : Speed vs. Flow (1/23/05 - 1/29/05)
NB 5
SB 5
sparse / fast
dense / slow
average speed
aggregate mainline 5-minute flow
0
10
20
30
40
50
60
70
80
90
0
100
200
300
400
500
600
700
800



Velocity - Flow relationship
Total Simulated Time 59.9917 min.
Total Simulated Time 1.6589 min.
τ_0=0.23, L=4, J_0=6
Total Periodic Distance 1 miles
Velocity (miles/hour).
Flow (veh./hour). 1-lane highway.
0
20
40
60
80
100
0
200
400
600
800
1000
1200
1400
1600
1800

Deterministic Closures

Recall the traffic flow model is, $\frac{d}{dt} Ef(\sigma) = EMf(\sigma)$ or

$$\frac{d}{dt} Ef(\sigma) = E\sum_{x\in\Lambda} c_0 \sigma(x)(1-\sigma(x+1))e^{-U(x,\sigma)}[f(\sigma^{x,x+1}) - f(\sigma)]$$

where $U(x,\sigma) = \sum_{\substack{z\neq x \\ z\in\Lambda}} J(x,z)\sigma(z)$

In particular we pick $f(\sigma) = \sigma(z)$ for some fixed z in L and we can simplify $f(\sigma^{x,x+1}) - f(\sigma)$ as follows

Since, $$\sigma^{x,x+1}(z) = \begin{cases} \sigma(z), & z \neq x, z \neq x+1 \\ \sigma(x+1), & z = x \\ \sigma(x), & z = x+1 \end{cases}$$

Then we have, $$f(\sigma^{x,x+1}) = \sigma^{x,x+1}(z) = \begin{cases} \sigma(z) & , \ x \neq z, x \neq z-1 \\ \sigma(z+1), & x = z \\ \sigma(z-1), & x = z-1 \end{cases}$$

and therefore, $$f(\sigma^{x,x+1}) - f(\sigma) = \begin{cases} 0 & , \ x \neq z, x \neq z-1 \\ \sigma(z+1) - \sigma(z), & x = z \\ \sigma(z-1) - \sigma(z), & x = z-1 \end{cases}$$

Deterministic Closures

Therefore $\frac{d}{dt} Ef(\sigma) = EMf(\sigma)$ becomes

$$\frac{d}{dt} E\sigma_t(z) = -Ec_0\sigma(z)(1-\sigma(z+1))e^{-U(z,\sigma)} + Ec_0\sigma(z-1)(1-\sigma(z))e^{-U(z-1,\sigma)}$$

where $U(x,\sigma) = \sum_{\substack{z \neq x \\ z \in \Lambda}} J(x,z)\sigma(z)$

Exact but not yet closed for $E\sigma_t(z) = \mathrm{Prob}(\sigma_t(z) = 1)$

Suppose that J has uniform (J=Jo), weak long interactions.

Finite Difference Scheme

The LLN formally applies and the fluctuations of $\sum_{y \neq x} J(y-x)\sigma(y)$ about their mean will be small.

Then in the long range interaction limit we have,

$$Ee^{-U(x,\sigma)} = Ee^{-\sum J(y-x)\sigma(y)} \overset{N,L\to\infty}{\approx} e^{-\sum J(y-x)E\sigma(y)} + o_N(1)$$

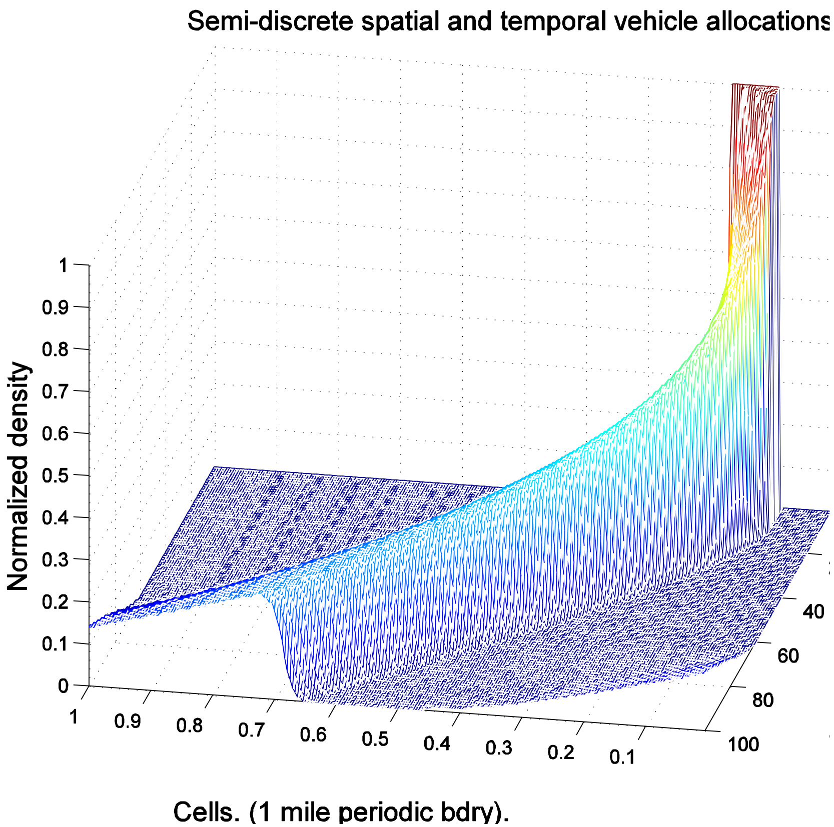
Let $u(z,t) = E\sigma_t(z)$ then we obtain an approximate *semi-discrete finite difference scheme*:

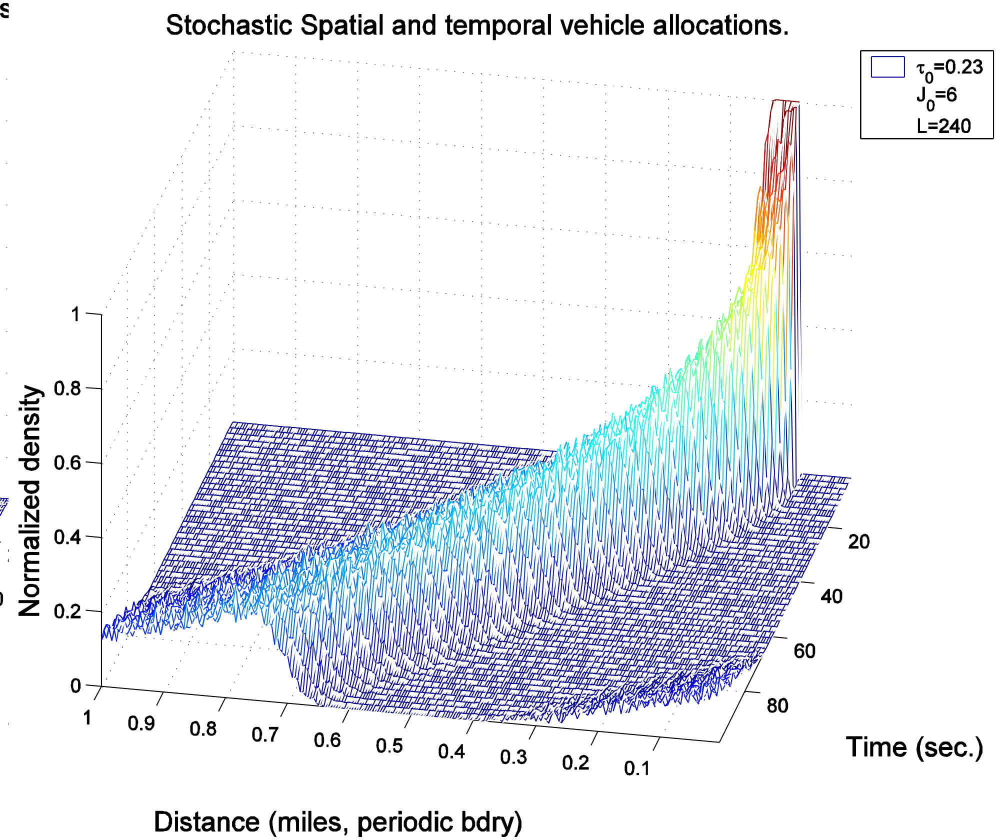
$$\boxed{\frac{d}{dt}u(z,t) + F(z+1,t) - F(z,t) = 0}$$

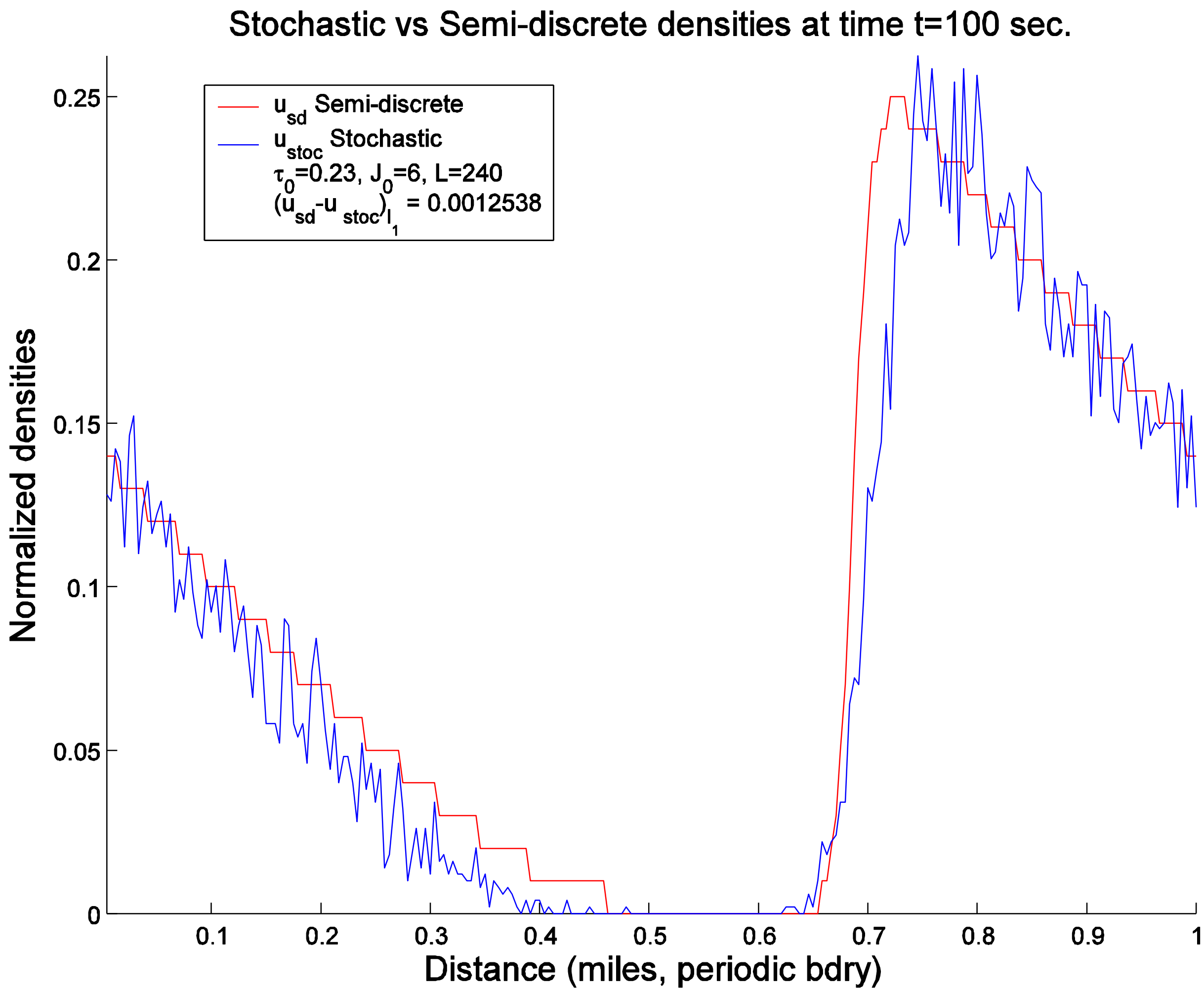
where $F(z,t) = c_0 u(z-1,t)(1-u(z,t))e^{-J\circ u(z-1,t)}$

For a periodic lattice this scheme is conservative.

Comparisons between semi-discrete scheme and microscopic stochastic model







Potential Radius L	240	100	50	10	4	1
l_1 Rel. Error	.0013	.0029	.0051	.0066	.0126	.02

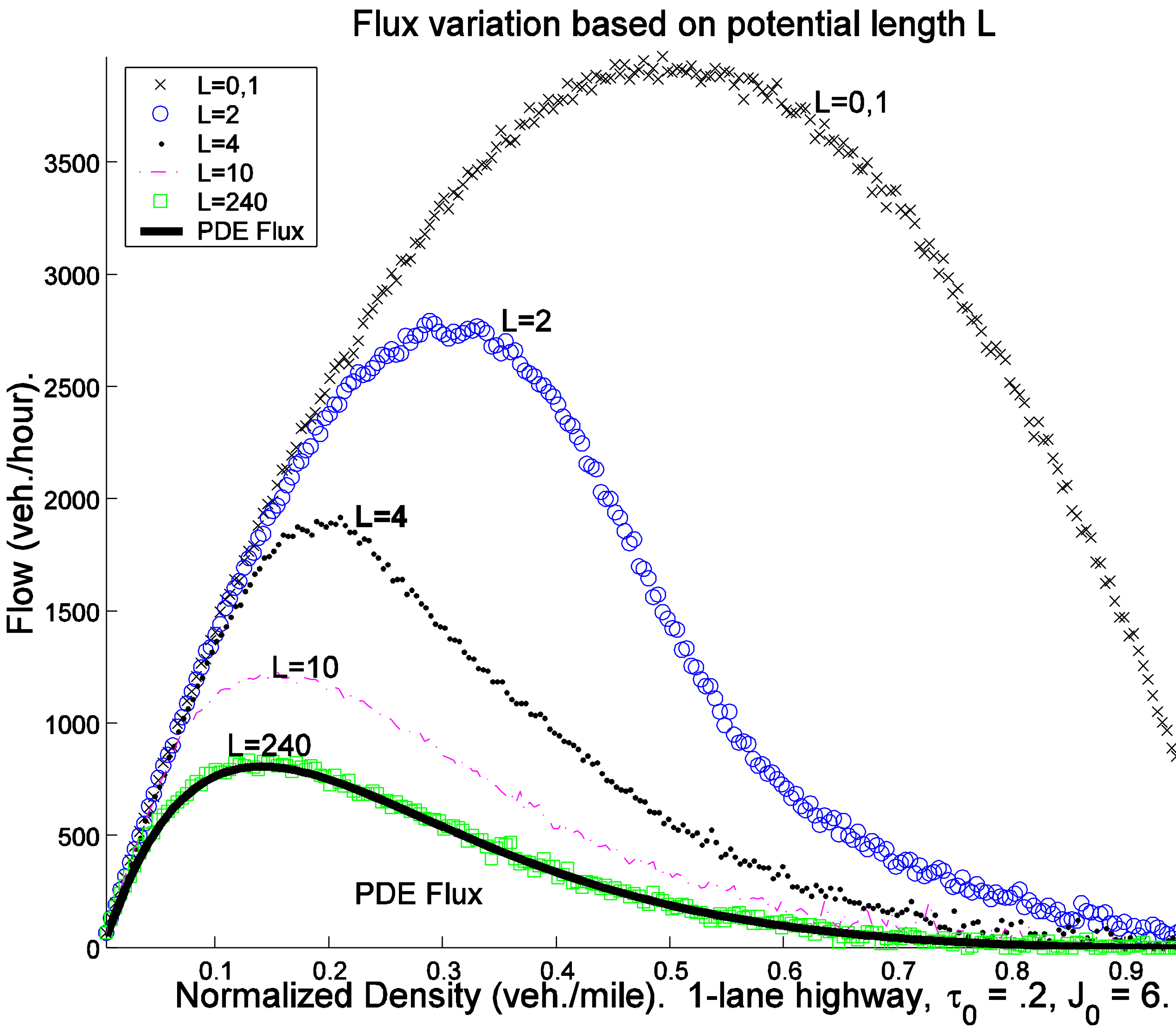
PDE model

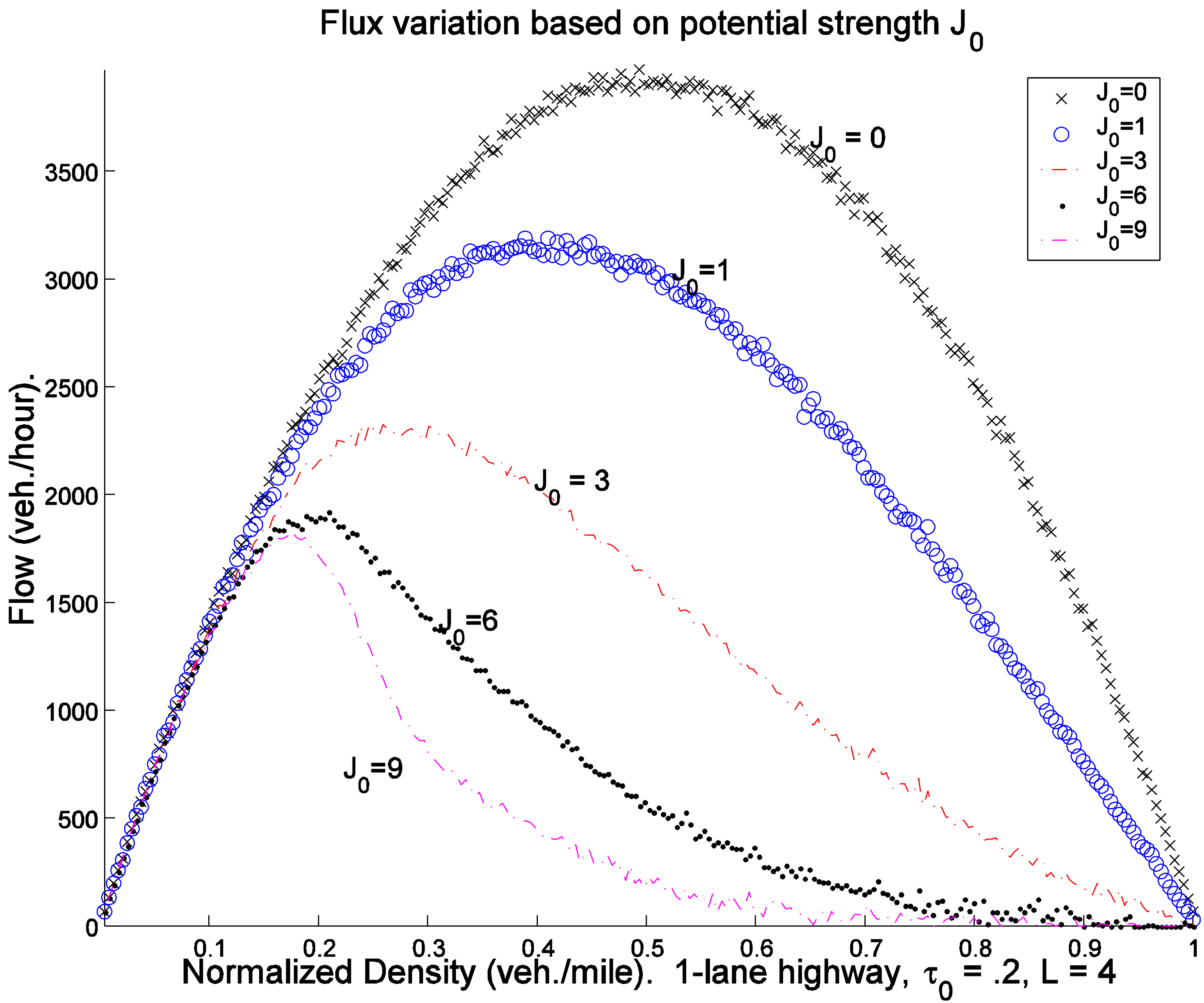
Expanding in Taylor we obtain, $\frac{d}{dt}u + [hc_0 u(1-u)e^{-J\circ u}]_z = O(h^2)$

Rescaling time via $t \to th^{-1}$ in order to absorb h and omiting the $O(h^2)$ term, we obtain the following macroscopic transport equation:

$$\boxed{u_t + F(u)_z = 0}$$

where the PDE flux is $F(u) = c_0 u(1-u)e^{-J\circ u}$


Flux variation based on potential length L
L=0,1
L=2
L=4
L=10
L=240
PDE Flux
3500
3000
2500
2000
1500
1000
500
0
Flow (veh./hour).
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
Normalized Density (veh./mile). 1-lane highway, τ_0 = .2, J_0 = 6.


Flux variation based on potential strength J0
Flow (veh./hour).
Normalized Density (veh./mile). 1-lane highway, τ0 = .2, L = 4
J0=0
J0=1
J0=3
J0=6
J0=9
J0 = 0
J0 =1
J0 = 3
J0=6
J0=9
0
500
1000
1500
2000
2500
3000
3500
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1

Hierarchical Comparisons

Expanding the convolution,

$$J \circ u = \int_z^\infty V(y-z)u(y)dy \overset{x=y-z}{=} \int_0^\infty V(x)u(x+z)dx = J_0 u + J_1 u_z + J_2 u_{zz} + \ldots$$

we can approximate the exponential via,

$$e^{-J\circ u} \approx e^{-J_0 u}[1 - J_1 u_z - J_2 u_{zz}]$$

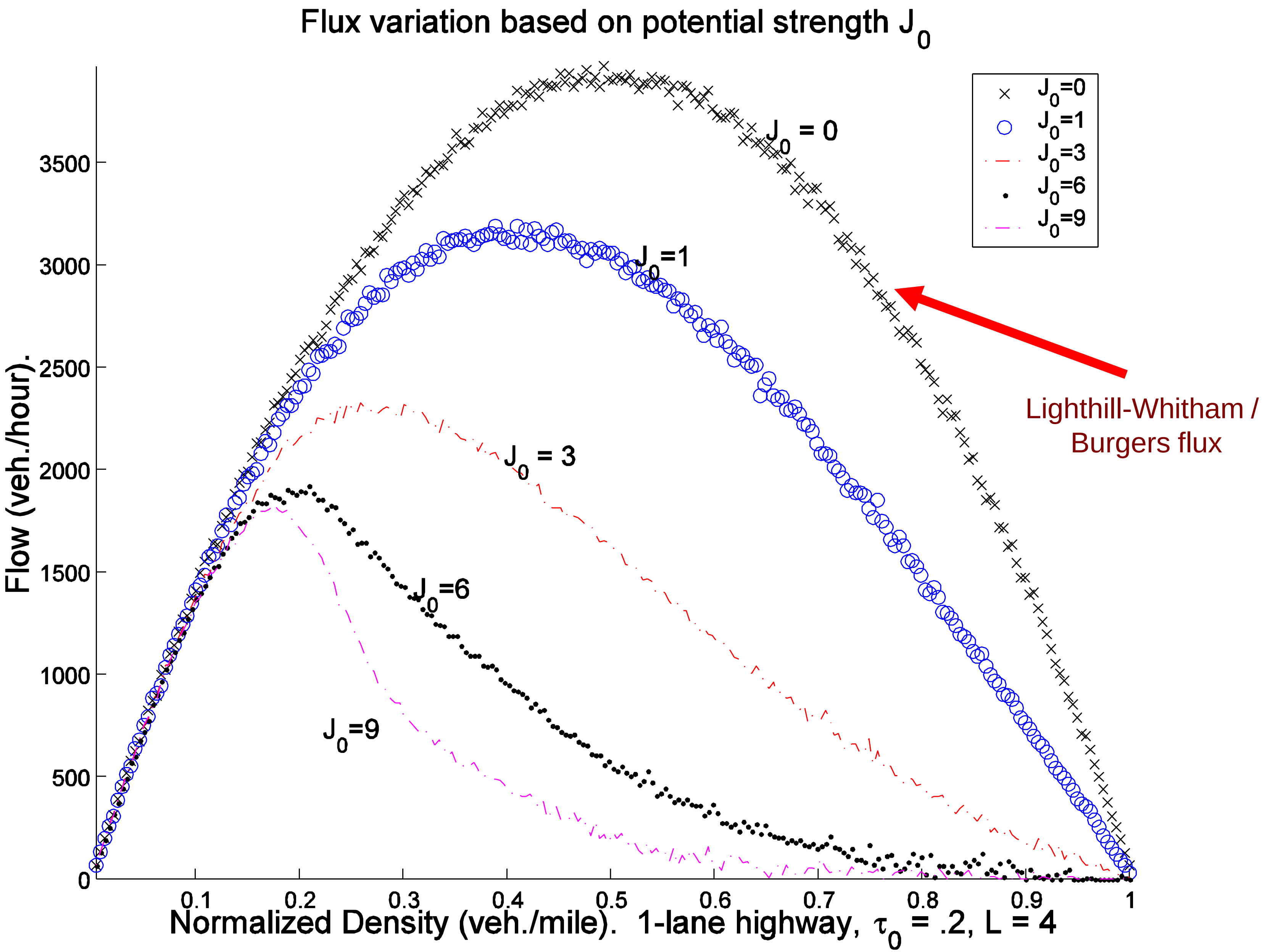
The traffic model PDE $u_t + cu(1-u)e^{-J\circ u} = 0$ therefore becomes…

The traffic model PDE,

$$u_t + c_0[u(1-u)e^{-J_0 u}]_z = c_0[J_1 u(1-u)e^{-J_0 u} u_z]_z + c_0[J_2 u(1-u)e^{-J_0 u} u_{zz}]_z$$

Note:

- No interactions (J=0):
  Lighhill-Whitham/Burger's eq. $\rightarrow u_t + c_0[u(1-u)]_z = 0$



Flux variation based on potential strength J_0
$J_0=0$
$J_0=1$
$J_0=3$
$J_0=6$
$J_0=9$
$J_0 = 0$
$J_0 =1$
$J_0 = 3$
$J_0 =6$
$J_0 =9$
Lighthill-Whitham / Burgers flux
Flow (veh./hour).
Normalized Density (veh./mile). 1-lane highway, τ_0 = .2, L = 4
0
500
1000
1500
2000
2500
3000
3500
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1

The traffic model PDE,

$$u_t + c_0[u(1-u)e^{-J_0 u}]_z = c_0[J_1 u(1-u)e^{-J_0 u} u_z]_z + c_0[J_2 u(1-u)e^{-J_0 u} u_{zz}]_z$$

Note:

- No interactions (J=0):
  Lighhill-Whitham/Burger's eq. $\rightarrow u_t + c_0 u(1-u) = 0$
- Long range (L=N) uniform (J=Jo) interactions:
  Non-local flux $\rightarrow u_t + c_0[u(1-u)e^{-J_0 \bar{u}}]_z = 0$
- Including terms up to Jo in the convolution,
  Non-convex flux $\rightarrow u_t + c_0[u(1-u)e^{-J_0 u}]_z = 0$
- Terms up to J_1
  Nonlinear diffusive LWR type
- Full model is higher order dispersive (KDV type?)
  with nonlinear coefficients

Multi-lane extensions

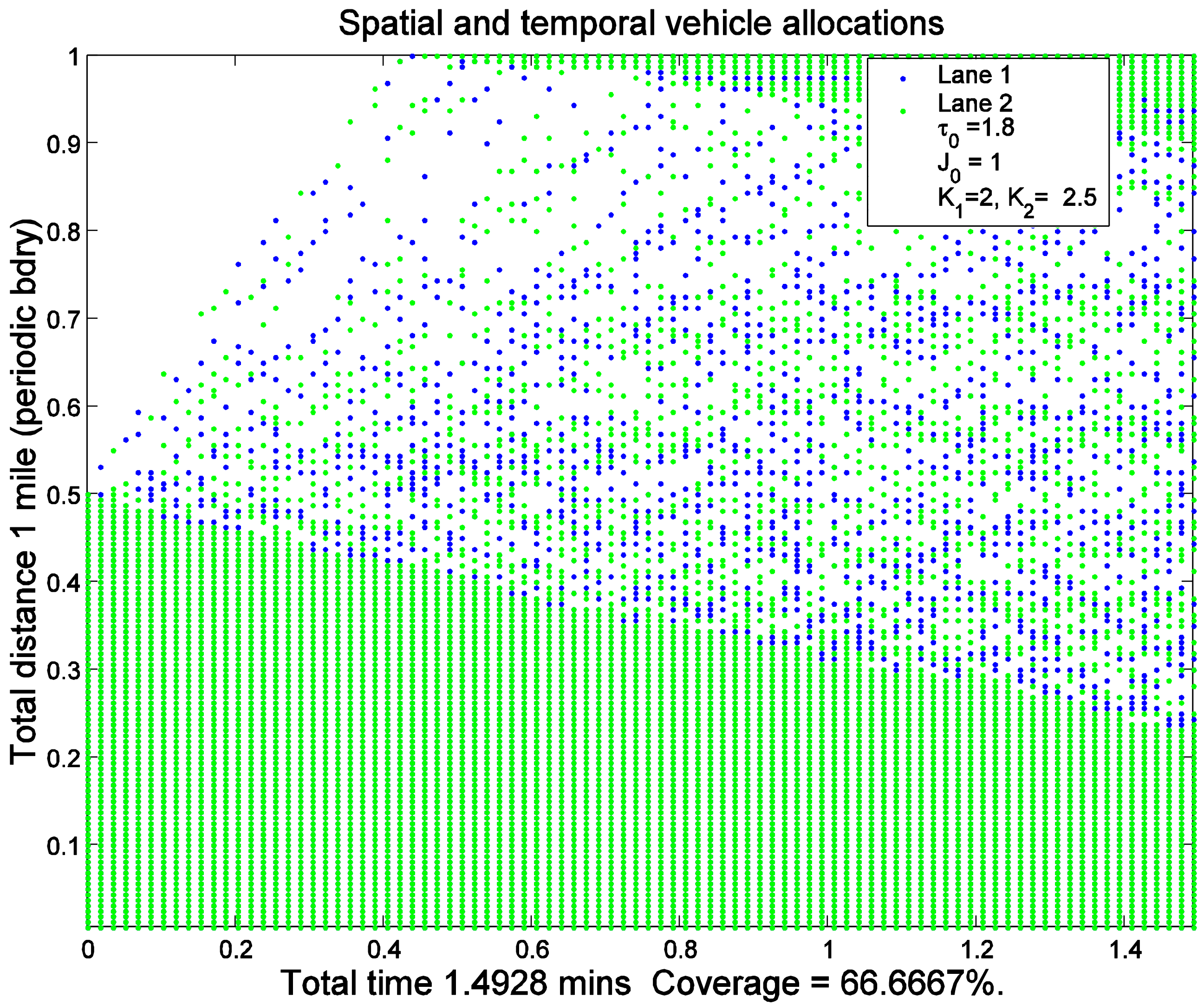
- We assume a two-dimensional domain (multi-lane highway).
- We introducing preferred direction in lane-changing via an anisotropy type potential. Thus our total interaction potential now consists of:

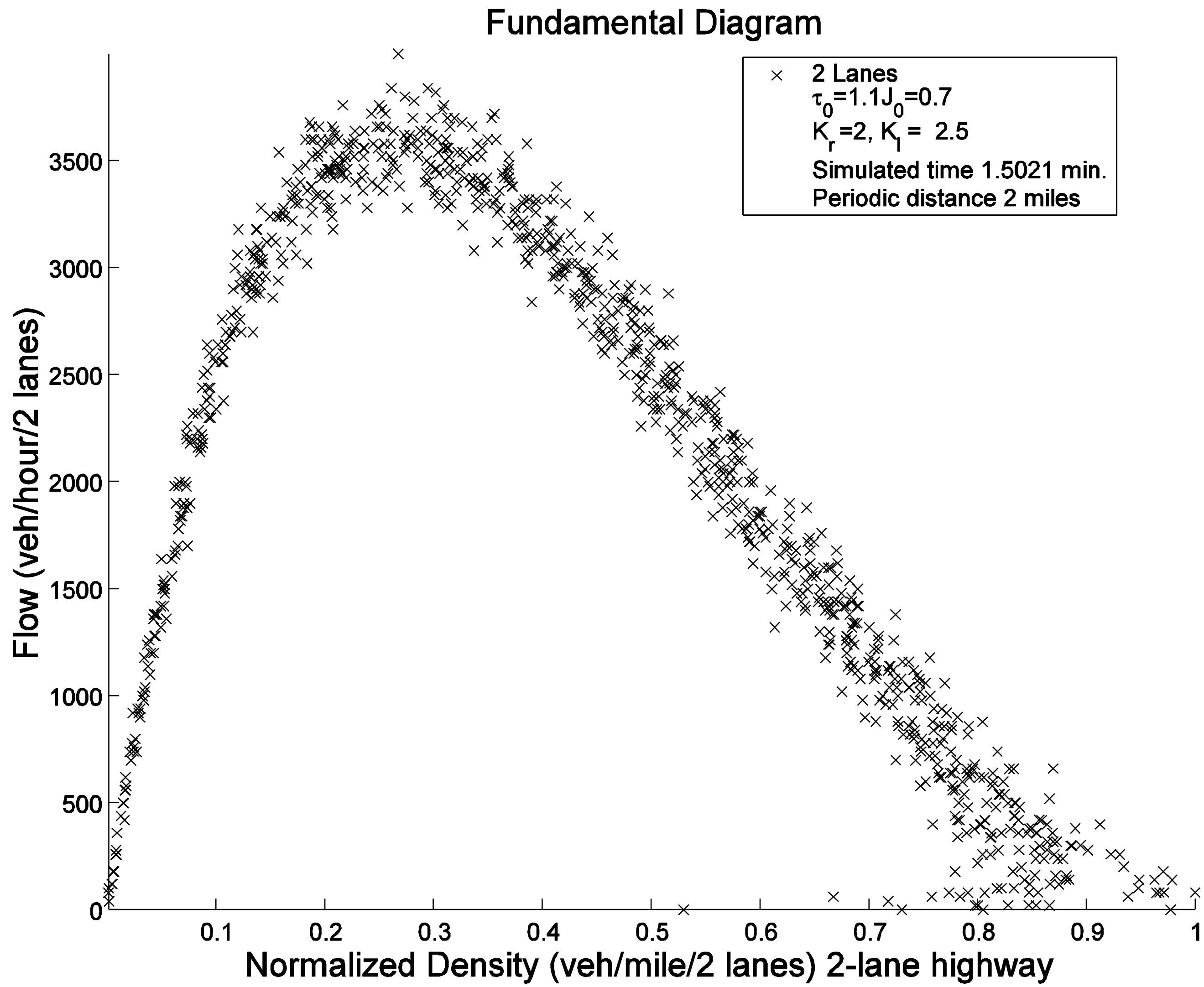
$$U(x) = U_e + U_a + h$$

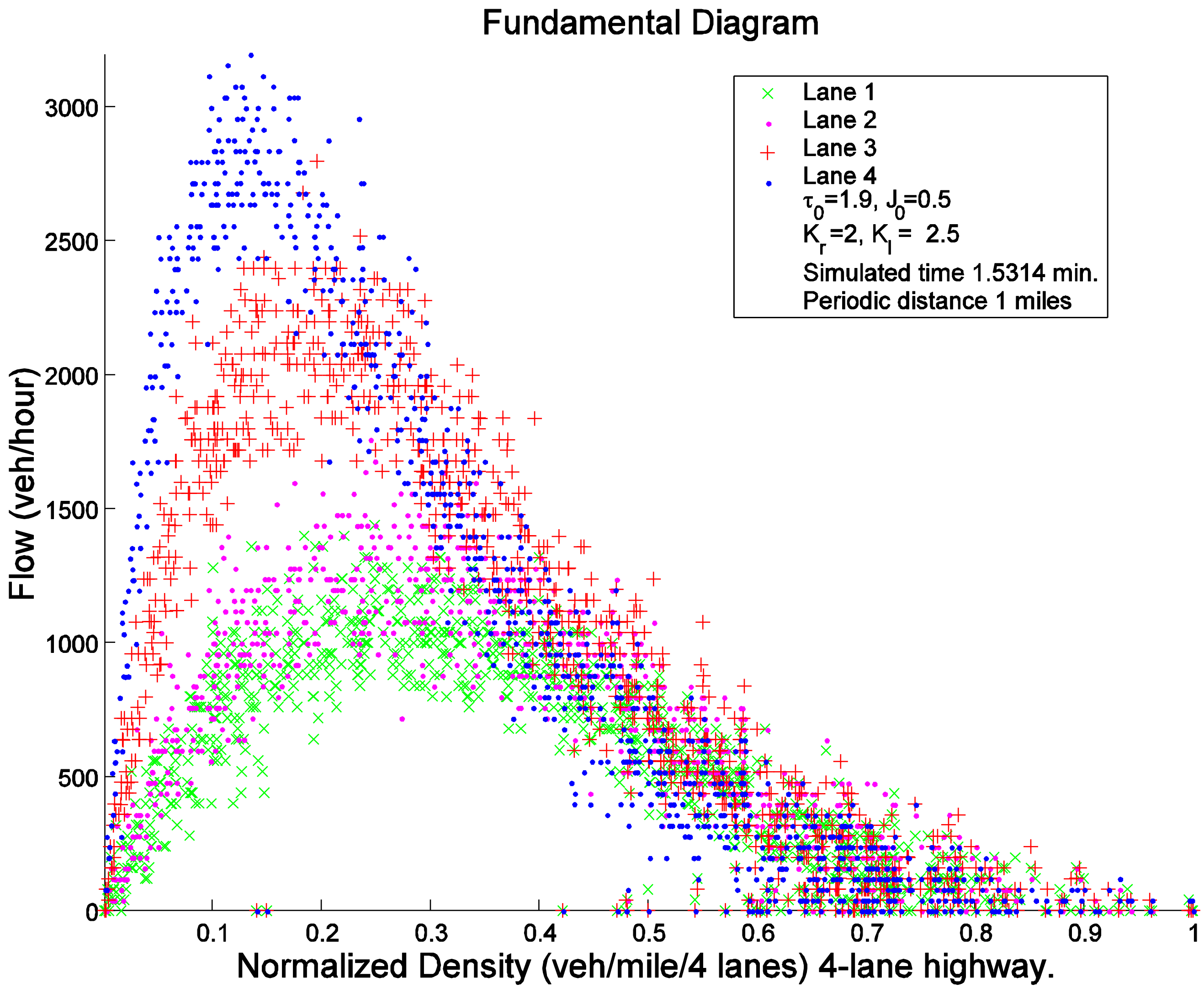
where $U_a(x) = \sum_{y=nn} \psi(x,y)$ with $\psi(x,y) = \begin{cases} k_l & \text{if } y = x+1 \\ k_r & \text{if } y = x-1 \\ k_f & \text{if } y = x+n \end{cases}$

- Calibrate parameters:

# of Lanes	1	2	3	4
τ_0	0.23	1.1	1.85	1.9
J_0	6	0.7	0.7	0.5
Desired Velocity (mph)	65	62	68	72
Upstream Velocity (mph)	-10	-11	-12	-9.6


Spatial and temporal vehicle allocations
Total distance 1 mile (periodic bdry)
Total time 1.4928 mins Coverage = 66.6667%.
Lane 1
Lane 2
τ_0 =1.8
J_0 = 1
K_1=2, K_2= 2.5
0
0.2
0.4
0.6
0.8
1
1.2
1.4
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1

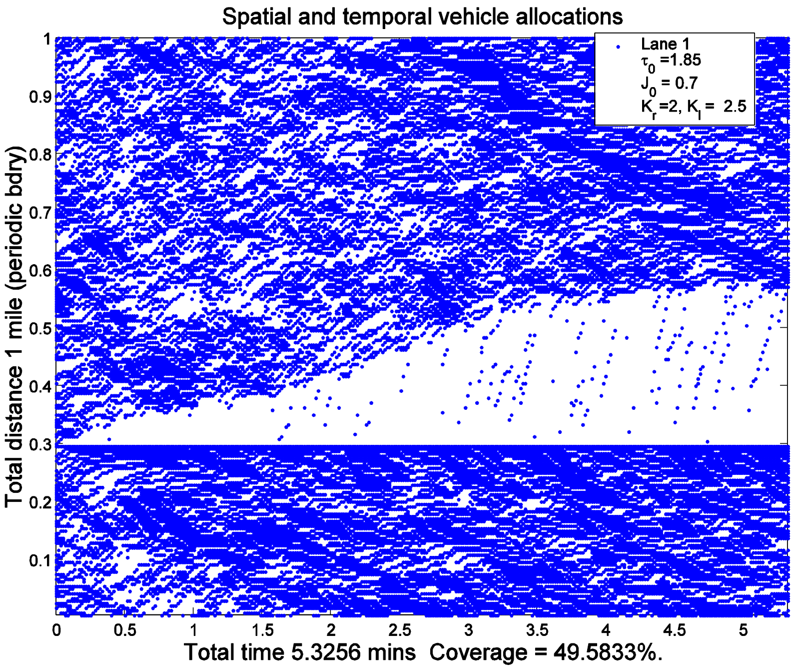

Fundamental Diagram
2 Lanes
τ0=1.1J0=0.7
Kr=2, Kl = 2.5
Simulated time 1.5021 min.
Periodic distance 2 miles
Flow (veh/hour/2 lanes)
0
500
1000
1500
2000
2500
3000
3500
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
Normalized Density (veh/mile/2 lanes) 2-lane highway

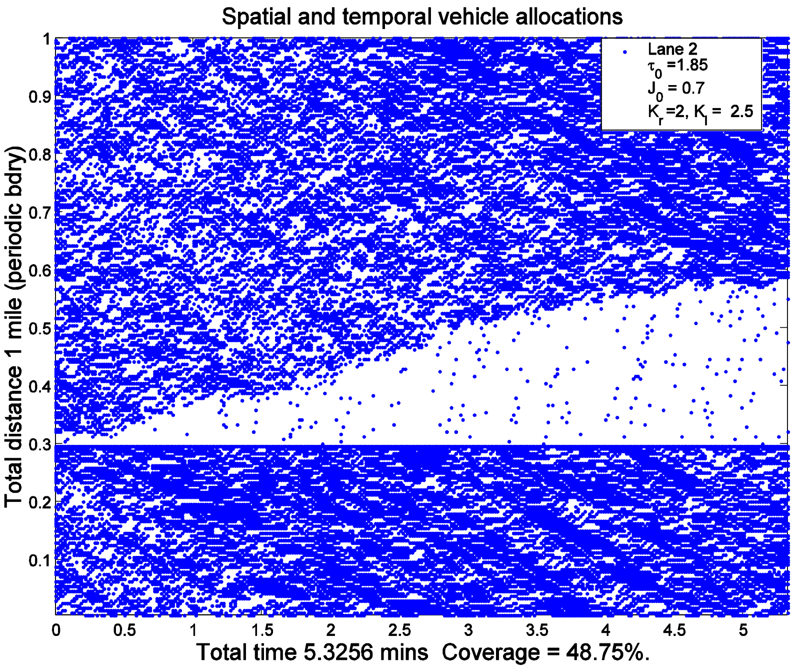


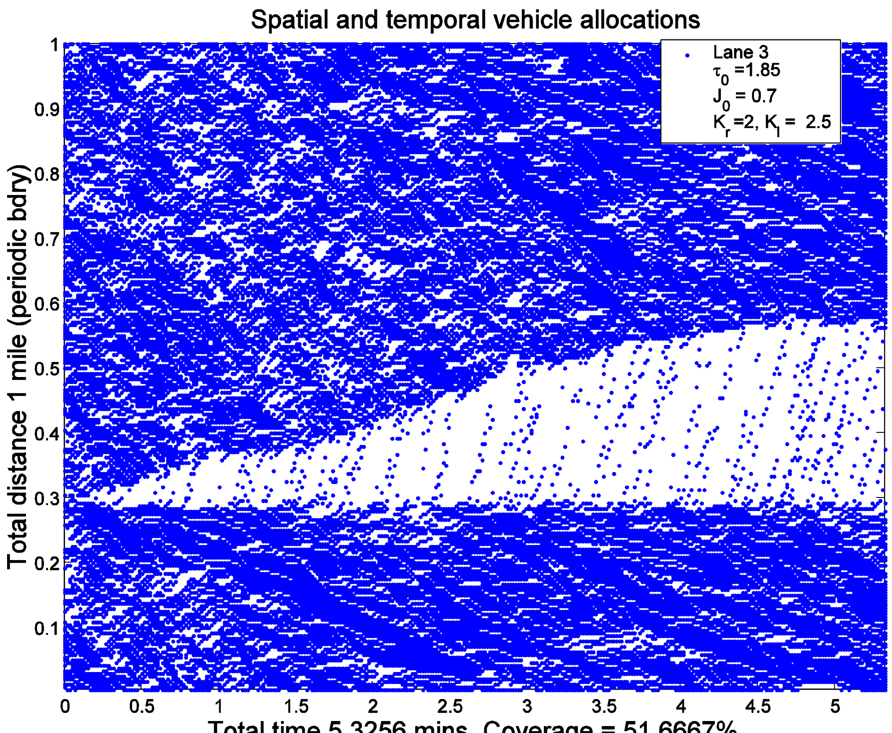
Fundamental Diagram
Lane 1
Lane 2
Lane 3
Lane 4
τ0=1.9, J0=0.5
Kr=2, Kl = 2.5
Simulated time 1.5314 min.
Periodic distance 1 miles
Flow (veh/hour)
0
500
1000
1500
2000
2500
3000
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
Normalized Density (veh/mile/4 lanes) 4-lane highway.

Test case toy problem: an incident

- Assume a 3-lane highway
- Let anisotropy coefficients: Kr=2, Kl=2.6, Kf=8
- Block lanes 1 and 2 (i.e. an accident)


Spatial and temporal vehicle allocations
Lane 1
τ_0 =1.85
J_0 = 0.7
K_r =2, K_l = 2.5
Total distance 1 mile (periodic bdry)
Total time 5.3256 mins Coverage = 49.5833%.


Spatial and temporal vehicle allocations
Lane 2
τ_0 =1.85
J_0 = 0.7
K_r =2, K_l = 2.5
Total distance 1 mile (periodic bdry)
Total time 5.3256 mins Coverage = 48.75%.


Spatial and temporal vehicle allocations
Lane 3
τ_0 =1.85
J_0 = 0.7
K_r =2, K_l = 2.5
Total distance 1 mile (periodic bdry)
Total time 5.3256 mins Coverage = 51.6667%.

Conclusions

- ✓ Presented a novel modeling approach based on microscopic Arrhenius spin-exchange dynamics
- ✓ Extended method to multi-lane traffic
- ✓ Studied deterministic closures of the microscopic stochastic model at different length scales
- ✓ Obtained formal hierarchical comparisons with other well-known models of traffic
- ✓ Presented Kinetic Monte Carlo simulations which allows for comparisons with actual traffic data as well as other PDE models

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