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PyMS version 1.0

A Python toolkit for processing of chromatography–mass spectrometry data

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Introduction

1.1 About PyMS

PyMS is a Python toolkit for processing of chromatography–mass spectrometry data. The main idea behind PyMS is to provide a framework and a set of components for rapid development and testing of methods for processing of chromatography–mass spectrometry data. An important objective of PyMS is to decouple processing methods from visualization and the concept of interactive processing. This is useful for high-throughput processing tasks and when there is a need to run calculations in the batch mode.

PyMS is modular and consists of several sub-packages written in Python programming language [1]. PyMS is released as open source, under the GNU Public License version 2.

There are four parts of the pyms project:

- pyms – The PyMS code
- pyms-docs – The PyMS documentation
- pyms-test – Examples of PyMS use

Each part is a separate project on Google Code that can be downloaded separately. The data used in PyMS documentation and examples is available from the Bio21 Institute server:

<http://bioinformatics.bio21.unimelb.edu.au/pyms-data/>

In addition, the current PyMS API documentation is available from here:

<http://bioinformatics.bio21.unimelb.edu.au/pyms.api/index.html>

1.2 PyMS installation

There are several ways to install PyMS depending your computer configuration and preferences. The recommended way install PyMS is to compile Python from sources and install PyMS within the local Python installation. This procedure is described below.

PyMS has been developed on Linux, and a detailed installation instructions for Linux are given below. Installation on any Unix-like system should be similar. We have not tested PyMS under Microsoft Windows.

1.2.1 Downloading PyMS source code

PyMS source code resides on Google Code servers, and can be accessed from the following URL: <http://code.google.com/p/pyms/>. Under the section "Source" one can find the instructions for downloading the source code. The same page provides the link under "This project's Subversion repository can be viewed in your web browser" which allows one to browse the source code on the server without actually downloading it.

Google Code maintains the source code with the program 'subversion' (an open-source version control system). To download the source code one needs to use the subversion client program called 'svn'. The 'svn' client exists for all mainstream operating systems¹, for more information see <http://subversion.tigris.org/>. The book about subversion is freely available on-line at <http://svnbook.red-bean.com/>. Subversion has extensive functionality. However only the very basic functionality is needed to download PyMS source code.

If the computer is connected to the internet and the subversion client is installed, the following command will download the latest PyMS source code:

```
$ svn checkout http://pyms.googlecode.com/svn/trunk/ pyms
A    pyms/Peak
A    pyms/Peak/__init__.py
A    pyms/Peak/List
A    pyms/Peak/List/__init__.py
.....
Checked out revision 71.
```

1.2.2 PyMS installation

PyMS installation consists of placing the PyMS code directory (pyms/) in place visible to Python interpreter. This can be in the standard place for 3rd party software (the directory site-packages/). If PyMS code is placed in a non-standard place the Python interpreter needs to be made aware of it before before it is possible to import PyMS modules (see the Python `sys.path.append()` command).

We recommend compiling your own Python installation for PyMS.

In addition to the PyMS core source code, a number of external packages is used to provide additional functionality. These are explained below.

¹For example, on Linux CentOS 4 we have installed the RPM package 'subversion-1.3.2-1.rhel4.i386.rpm' to provide us with the subversion client 'svn'.

1.2.3 Package 'NumPy'

The package NumPy provides numerical capabilities to Python. This package is used throughout PyMS (and also required for some external packages used in PyMS), so its installation is mandatory.

The NumPy web site <http://numpy.scipy.org/> provides the installation instructions and the link to the source code.

1.2.4 Package 'pycdf' (required for reading ANDI-MS files)

The pycdf (a python interface to Unidata netCDF library) source and installation instructions can be downloaded from <http://pysclint.sourceforge.net/pycdf/>. Follow the installation instructions to install pycdf.

1.2.5 Package 'Pycluster' (required for peak alignment by dynamic programming)

The peak alignment by dynamic programming is located in the subpackage `pymms.Peak.List.DPA`. This subpackage uses the Python package 'Pycluster' as the clustering engine. Pycluster with its installation instructions can be found here: <http://bonsai.ims.u-tokyo.ac.jp/~mdehoon/software/cluster/index.html>.

1.2.6 Package 'scipy.ndimage' (required for TopHat baseline corrector)

If the full SciPy package is installed the 'ndimage' will be available. However the SciPy contains large amount of functionality, and its installation is somewhat involved. In some situations it may be preferable to install only the subpackage 'ndimage'. The UrbanSim web site [2] provides instructions how to install a local copy of 'ndimage'. These instructions and the link to the file 'ndimage.zip' are here: <http://www.urbansim.org/opus/releases/opus-4-1-1/docs/installation/scipy.html>

1.3 Current PyMS development environment

PyMS is currently being developed with the following packages:

```
Python-2.5.2
numpy-1.1.1
netcdf-4.0
pycdf-0.6-3b
Pycluster-1.41
```

A quick installation guide for packages required by PyMS is given below.

1. Python installation:

```
$ tar xvfz Python-2.5.2.tgz
$ cd Python-2.5.2
$ ./configure
$ make
$ make install
```

This installs python in /usr/local/lib/python2.5. Make sure that python called from the command line is the one just compiled and installed.

2. NumPy installation:

```
$ tar xvfz numpy-1.1.1.tar.gz
$ cd numpy-1.1.1
$ python setup.py install
```

3. pycdf installation

Pycdf has two dependencies: the Unidata netcdf library and NumPy. The NumPy installation is described above. To install pycdf, the netcdf library must be downloaded (<http://www.unidata.ucar.edu/software/netcdf/>) compiled and installed first:

```
$ tar xvfz netcdf.tar.gz
$ cd netcdf-4.0
$ ./configure
$ make
$ make install
```

The last step will create several binary 'libnetcdf*' files in /usr/local/lib. pycdf can be installed as follows:

```
$ tar xvfz pycdf-0.6-3b
$ cd pycdf-0.6-3b
$ python setup.py install
```

4. Pycluster installation

```
$ tar xvfz Pycluster-1.42.tar.gz
$ cd Pycluster-1.42
$ python setup.py install
```

5. ndimage installation:

```
$ unzip ndimage.zip
$ cd ndimage
$ python setup.py install --prefix=/usr/local
```

Since ndimage was installed outside the scipy package, this requires some manual correction:

```
$ cd /usr/local/lib/python2.5/site-packages
$ mkdir scipy
$ touch scipy/__init__.py
$ mv ndimage scipy
```

1.4 Troubleshootings

The PyMS is essentially a python library (a 'package' in python parlance, which consists of several 'sub-packages'), which for some functionality depends on other python libraries, such as NumPy, pycdf, and Pyccluster. The most likely problem with PyMS installation is a problem with installing one of the PyMS dependencies.

1.4.1 Pycdf import error

On Red Hat Linux 5 the SELinux is enabled by default, and this causes the following error while trying to import properly installed pycdf:

```
$ python
Python 2.5.2 (r252:60911, Nov  5 2008, 16:25:39)
[GCC 4.1.1 20070105 (Red Hat 4.1.1-52)] on linux2
Type "help", "copyright", "credits" or "license" for more information.
>>> import pycdf
Traceback (most recent call last):
  File "<stdin>", line 1, in <module>
  File "/usr/local/lib/python2.5/site-packages/pycdf/__init__.py", line 22, in <module>
    from pycdf import *
  File "/usr/local/lib/python2.5/site-packages/pycdf/pycdf.py", line 1096, in <module>
    import pycdfext as _C
  File "/usr/local/lib/python2.5/site-packages/pycdf/pycdfext.py", line 5, in <module>
    import _pycdfext
ImportError: /usr/local/lib/python2.5/site-packages/pycdf/_pycdfext.so:
  cannot restore segment prot after reloc: Permission denied
```

This problem is removed simply by disabling SELinux (login as 'root', open the menu Administration → Security Level and Firewall, tab SELinux, change settings from 'Enforcing' to 'Disabled').

This problem is likely to occur on Red Hat Linux derivative distributions such as CentOS.

1.5 PyMS tutorial and examples

A tutorial illustrating various PyMS features is provided in subsequent chapter of this User Guide. The commands executed interactively are grouped together by example, and provided as Python scripts in the project 'pym-test' (this is a Google code project, similar to the project 'pym' which contains the PyMS source code).

The setup used in the examples below is as follows. The projects 'pym', 'pym-test', 'pym-docs', and 'data' are all in the same directory, '/x/PyMS'. In the project 'pym-test' there is a directory corresponding to each example coded with the example number (ie. `pym-test/21a/` corresponds to Example 1a in Chapter 2).

In each example directory, there is a script named 'proc.py' which contains the commands given in the example. Provided that the paths to 'pym' and 'pym-data' are set properly, these scripts could be run with the following command:

```
$ python proc.py
```

Before running each example the Python interpreter was made aware of the PyMS location with the following commands:

```
import sys
sys.path.append("/x/PyMS")
```

For brevity these commands will not be shown in the examples below, but they are included in 'pym-test' example scripts. The above path may need to be adjusted to match your own directory structure.

All data files (raw data files, peak lists etc.) used in the example below can be found at <http://bioinformatics.bio21.unimelb.edu.au/pym/data/> and are assumed to be located in the 'data' directory.

GC-MS Raw Data Model

2.1 Introduction

PyMS can read gas chromatography-mass spectrometry (GC-MS) data stored in Analytical Data Interchange for Mass Spectrometry (ANDI-MS),² and Joint Committee on Atomic and Molecular Physical Data (JCAMP-DX)³ formats. These formats are essentially recommendations, and it is up to individual vendors of mass spectrometry processing software to implement “export to ANDI-MS” or “export to JCAMP-DX” features in their software. It is also possible to get third party converters. The information contained in the exported data files can vary significantly, depending on the instrument, vendor’s software, or conversion utility.

For PyMS, the minimum set of assumptions about the information contained in the data file are:

- The data contain the m/z and intensity value pairs across a scan.
- Each scan has a retention time.

Internally, PyMS stores the raw data from ANDI files or JCAMP files as a `GCMS_data` object. Once a `GCMS_data` object has been created, the raw data can not be modified.

2.2 Reading the raw GC-MS data

2.2.1 Reading JCAMP GC-MS data

[*This example is in `pyms-test/20a`*]

The PyMS package `pyms.GCMS.IO.JCAMP` provides capabilities to read the raw GC-MS data stored in the JCAMP-DX format.

The file ‘gc01_0812_066.jdx’ (located in ‘data’) is a GC-MS experiment converted from Agilent ChemStation format to JCAMP format using File Translator Pro.⁴ This file can be loaded in Python as

²ANDI-MS was developed by the Analytical Instrument Association.

³JCAMP-DX is maintained by the International Union of Pure and Applied Chemistry.

⁴ChemSW, Inc.

follows:

```
>>> from pyms.GCMS.IO.JCAMP.Function import JCAMP_reader
>>> jcamp_file = "/x/PyMS/data/gc01_0812_066.jdx"
>>> data = JCAMP_reader(jcamp_file)
-> Reading JCAMP file '/x/PyMS/pyms-data/gc01_0812_066.jdx'
>>>
```

The above command creates the object ‘data’ which is an *instance* of the class `GCMS_data`.

2.2.2 Reading ANDI GC-MS data

[*This example is in pyms-test/20b*]

The PyMS package `pyms.GCMS.IO.ANDI` provides capabilities to read the raw GC-MS data stored in the ANDI-MS format.

The file ‘gc01_0812_066.cdf’ (located in ‘data’) is a GC-MS experiment converted to ANDI-MS format from Agilent ChemStation (from the same data as in example 20a above). This file can be loaded as follows:

```
>>> from pyms.GCMS.IO.ANDI.Function import ANDI_reader
>>> ANDI_file = "/x/PyMS/data/gc01_0812_066.cdf"
>>> data = ANDI_reader(ANDI_file)
-> Reading netCDF file '/x/PyMS/pyms-data/gc01_0812_066.cdf'
>>>
```

The above command creates the object ‘data’ which is an *instance* of the class `GCMS_data`.

2.3 A GCMS_data object

2.3.1 Methods

[*The following examples are the same in pyms-test/20a and pyms-test/20b*]

The object ‘data’ (from the two previous examples) stores the raw data as a *GCMS_data* object. Within the `GCMS_data` object, raw data are stored as a list of *Scan* objects and a list of retention times. There are several methods available to access data and attributes of the `GCMS_data` and *Scan* objects.

The `GCMS_data` object’s methods relate to the raw data. The main properties relate to the masses, retention times and scans. For example, the minimum and maximum mass from all of the raw data can be returned by the following:

```
>>> data.get_min_mass()
>>> data.get_max_mass()
```

A list of all retention times can be returned by:

```
>>> time = data.get_time_list()
```

The index of a specific retention time (in seconds) can be returned by:

```
>>> data.get_index_at_time(400.0)
```

Note that this returns the index of the retention time in the data closest to the given retention time of 400.0 seconds.

The method `get_tic()` returns a total ion chromatogram (TIC) of the data as an `IonChromatogram` object:

```
>>> tic = data.get_tic()
```

The `IonChromatogram` object is explained in a later chapter.

2.3.2 Exploring a Scan data object

A `Scan` object contains a list of masses and a corresponding list of intensity values from a single mass-spectrum scan in the raw data. Typically only non-zero (or non-threshold) intensities and corresponding masses are stored in the raw data.

[*The following examples are the same in `pymms-test/20a` and `pymms-test/20b`*]

A list of all the raw `Scan` objects can be returned by:

```
>>> scans = data.get_scan_list()
```

A list of all masses in a scan (i.e. the 1st scan) is returned by:

2.3.3 A Scan data object

[*The following examples are the same in `pymms-test/20a` and `pymms-test/20b`*]

A `Scan` object contains a list of masses and a corresponding list of intensity values from a single mass-spectrum scan.

A list of all masses in a scan (e.g. the 1st scan) is returned by:

```
>>> scans[0].get_mass_list()
```

A list of all corresponding intensities in a scan is returned by:

```
>>> scans[0].get_intensity_list()
```

The minimum and maximum mass in an individual scan (i.e. the 1st scan) are returned by:

```
>>> scans[0].get_min_mass()
```

```
>>> scans[0].get_max_mass()
```

2.3.4 Exporting data and printing information about a data set

[*This example is in `pymms-test/20w`*]

Often it is of interest to find out some basic information about the data set, ie. the number of scans, the retention time range, and m/z range and so on. The GCMS_data class provides a method `info()` that can be used for this purpose.

```
>>> from pymms.GCMS.IO.ANDI.Function import ANDI_reader
>>> andi_file = "/x/PyMS/data/gc01_0812_066.cdf"
>>> data = ANDI_reader(andi_file)
-> Reading netCDF file '/x/PyMS/data/gc01_0812_066.cdf'
>>> data.info()
Data retention time range: 5.093 min -- 66.795 min
Time step: 0.375 s (std=0.000 s)
Number of scans: 9865
Minimum m/z measured: 50.000
Maximum m/z measured: 599.900
Mean number of m/z values per scan: 56
Median number of m/z values per scan: 40
>>>
```

To export the entire raw data to a file, use the method `write()`:

```
>>> data.write("output/data")
-> Writing intensities to 'output/data.I.csv'
-> Writing m/z values to 'output/data.mz.csv'
```

This method takes the string ("output/data", in this example) and writes two CSV files. One has extension ".I.csv" and contains the intensities ('output/data.I.csv' in this example), and the other has the extension ".mz" and contains the corresponding table of m/z value ("output/data.mz.csv" in this example). In general these are not two-dimensional matrices, because different scans may have different number of m/z values recorded.

2.3.5 Comparing two GC-MS data sets

[*This example is in `pyms-test/20x`*]

Occasionally it is useful to compare two data sets. For example, one may want to check the consistency between the data set exported in netCDF format from the manufacturer's software, and the JCAMP format exported from a third party software.

For example:

```
>>> from pyms.GCMS.IO.JCAMP.Function import JCAMP_reader
>>> from pyms.GCMS.IO.ANDI.Function import ANDI_reader
>>> andi_file = "/x/PyMS/data/gc01_0812_066.cdf"
>>> jcamp_file = "/x/PyMS/data/gc01_0812_066.jdx"
>>> data1 = ANDI_reader(andi_file)
-> Reading netCDF file '/x/PyMS/data/gc01_0812_066.cdf'
>>> data2 = JCAMP_reader(jcamp_file)
-> Reading JCAMP file '/x/PyMS/data/gc01_0812_066.jdx'
```

To compare the two data sets:

```
>>> from pyms.GCMS.Function import diff
>>> diff(data1,data2)
Data sets have the same number of time points.
Time RMSD: 1.80e-13
Checking for consistency in scan lengths ... OK
Calculating maximum RMSD for m/z values and intensities ...
Max m/z RMSD: 1.03e-05
Max intensity RMSD: 0.00e+00
```

If the data is not possible to compare, for example because of different number of scans, or inconsistent number of m/z values in between two scans, `diff()` will report the difference. For example:

```
>>> data2.trim(begin=1000,end=2000)
Trimming data to between 1000 and 2000 scans
>>> diff(data1,data2)
-> The number of retention time points different.
First data set: 9865 time points
Second data set: 1001 time points
Data sets are different.
```


GC-MS data derived objects

In this chapter the methods for converting the raw GC-MS data to an Intensity Matrix object are illustrated.

In the raw GC-MS data, consecutive scans do not necessarily contain the same mass per charge (mass) values. For data processing, it is often necessary to convert the data to a matrix with a set number of masses and scans. In PyMS there are functions to explicitly convert the raw mass values to consistent values across all scans.

3.1 IntensityMatrix Object

The general scheme for converting raw mass values is to bin intensity values based on the interval the corresponding mass belongs to. The general procedure is as follows:

- for a given bin size
- calculate the number of bins to cover the range of all masses.
- centre the first bin at the minimum mass found for all the raw data.
- sum intensities whose masses are in a given bin.

A mass, m , is considered to belong to a bin when $c - w/2 \leq m < c + w/2$, where c is the centre of the bin, and w is the width of the bin.

A function to bin masses to the nearest integer is also available.

Figure 3.1 illustrates the process of assigning bins to the mass axis and summing all intensities in a given bin. The result is a new mass axis with mass values corresponding to the centre of each bin.

[*This example is in `pymms-test/30`*]

An intensity matrix on the raw GCMS data can be built using the following functions. First the raw data is imported as before.

```
>>> from pymms.GCMS.IO.JCAMP.Function import JCAMP_reader
```

Figure 3.1: Mass intensity values are added to bins based on a pre-set bin size and the minimum mass of all the scan data. All intensities in a given bin width (top) are added and given a mass of the centre of the bin (bottom). For integer binning, each bin has a width of one and is centred at integer values.

```
>>> jcamp_file = "/x/PyMS/data/gc01_0812_066.jdx"
>>> data = JCAMP_reader(jcamp_file)
-> Reading JCAMP file '/x/PyMS/pyms-data/gc01_0812_066.jdx'
>>>
```

Then the data can be converted to an intensity matrix using the functions available in “pyms.GCMS.Functions”, namely `build_intensity_matrix()` and `build_intensity_matrix_i()`.

The default operation of `build_intensity_matrix()` is to use a bin size of one and treat the masses as floating point numbers. The default intensity matrix can be built as follows:

```
>>> from pyms.GCMS.Function import build_intensity_matrix
>>> im = build_intensity_matrix(data)
```

The size as the number of scans and the number of bins is returned by:

```
>>> im.get_size()
```

There are 9865 scans, 551 bins in this example.

The raw masses have been binned into new mass units based on the minimum mass in the raw data and the bin size. A list of the new masses are returned by:

```
>>> masses = im.get_mass_list()
```

It is also possible to search for a particular mass, by finding the index of the binned mass closest to the desired mass. For example, the index of the closest binned mass to a mass of 73.3 m/z is returned by:

```
>>> index = im.get_index_of_mass(73.3)
```

The value of the closest mass can be returned by indexing into the mass list:

```
>>> print masses[index]
```

A mass of 73.0 is returned in this example.

The bin size can be set values other than one. For example, the bin size can be set to 0.5.

```
im = build_intensity_matrix(data, 0.5)
```

The size of the intensity matrix will reflect the change in the number of bins.

```
>>> im.get_size()
```

There are 9865 scans (as before) and 1101 bins in this example.

The index and binned mass of the mass closest to 73.3 should also reflect the different binning.

```
>>> masses = im.get_mass_list()
>>> index = im.get_index_of_mass(73.3)
>>> print masses[index]
```

A mass of 73.5 is returned in this example.

It is also possible to build an intensity matrix with masses rounded to the nearest integer using a bin size of one. The function is imported from “pym.s.GCMS.Functions”.

```
>>> from pym.s.GCMS.Function import build_intensity_matrix_i
>>> im = build_intensity_matrix_i(data)
```

The masses are now all integers.

```
>>> masses = im.get_mass_list()
>>> index = im.get_index_of_mass(73.3)
>>> print masses[index]
```

A mass of 73 is returned in this example.

3.2 MassSpectrum Object

3.3 IonChromatogram Object

An IonChromatogram object is a one dimensional vector containing mass intensities as a function of retention time. This can be either m/z channel intensities (for example, ion chromatograms at m/z = 65), or cumulative intensities over all measured m/z (TIC).

An ion chromatogram object has a method `is_tic()` which returns True if the ion chromatogram is TIC, False otherwise:

```
>>> print "'tic' is a TIC:", tic.is_tic()
```

```
'tic' is a TIC: True
>>> print "'ic' is a TIC:",ic.is_tic()
'ic' is a TIC: False
```

3.3.1 Writing data to a file

The method `write()` of `IonChromatogram` object allows one to save the ion chromatogram object to a file:

```
>>> tic.write("output/tic.dat", minutes=True)
>>> ic.write("output/ic.dat", minutes=True)
```

The flag `minutes=True` indicates that retention time will be saved in minutes. The ion chromatogram object saved with the `write` method is a plain ASCII file which contains a pair of (retention time, intensity) per line:

```
$ head tic.dat
5.0944      745997.0000
5.1002      726566.0000
5.1059      717704.0000
5.1116      684214.0000
5.1173      701866.0000
5.1230      893306.0000
5.1287     1278099.0000
5.1345     1290984.0000
5.1402      925558.0000
5.1459      644122.0000
```

Figure 3.2 shows the plot of the file 'tic.dat' produced with the program Gnuplot. The Gnuplot script used to produce this plot is provided as `pym-s-test/01/output/plot.gnu`.

Figure 3.2: The Gnuplot plot of the file 'tic.dat'

3.4 Saving data

Data pre-processing

5.1 Noise smoothing

The purpose of noise smoothing is to remove high-frequency noise from data, and thereby increase the contribution of the signal relative to the contribution of the noise.

5.1.1 Window averaging

[*This example is in `pymms-test/51a`*]

A simple approach to noise smoothing is moving average window smoothing. In this approach the window of a fixed size ($2N + 1$ points) is moved across the ion chromatogram, and the intensity value at each point is replaced with the mean intensity calculated over the window size. The example below illustrates smoothing of TIC by window averaging.

Load the data and get the TIC:

```
>>> andi_file = "/x/PyMS/data/gc01_0812_066.cdf"
>>> data = ANDI_reader(andi_file)
-> Reading netCDF file '/x/PyMS/data/gc01_0812_066.cdf'
>>> tic = data.get_tic()
```

Apply the mean window smoothing with the 5-point window:

```
from pymms.Noise.SavitzkyGolay import window_smooth
tic1 = window_smooth(tic, window=5)
-> Window smoothing (mean): the wing is 2 point(s)
```

Apply the median window smoothing with the 5-point window:

```
>>> tic2 = window_smooth(tic, window=5, median=True)
-> Window smoothing (median): the wing is 2 point(s)
```

Apply the mean windows smoothing, but specify the window as a time string (in this example, 7 seconds):

```
>>> tic3 = window_smooth(tic, window='7s')
-> Window smoothing (mean): the wing is 9 point(s)
```

Time strings are explained in the Section 5.2.

5.1.2 Savitzky–Golay noise filter

[*This example is in `pyms-test/51b`*]

A more sophisticated noise filter is the Savitzky-Golay filter. Given the data loaded as above, this filter can be applied as follows:

```
>>> from pyms.Noise.SavitzkyGolay import savitzky_golay
>>> tic1 = savitzky_golay(tic)
-> Applying Savitzky-Golay filter
    Window width (points): 7
    Polynomial degree: 2
```

In this example the default parameters were used.

5.2 Time strings

A time string is specification of time interval, that takes the format 'NUMBERS' or 'NUMBERm' for time interval in seconds or minutes. For example, these are valid time strings: '10s' (10 seconds) and '0.2m' (0.2 minutes).

Bibliography

- [1] Python. <http://www.python.org>.
- [2] UrbanSim. <http://www.urbansim.org/>.

