

UniDyn--Demo-01.nb

John A. Marohn
jam99@cornell.edu
Cornell University

Abstract: This demonstration notebook loads the **UniDyn** package and executes the package's unit tests.

Set the path to the package

Tell *Mathematica* the path to the directory containing the packages. For the `$NCPath` variable, put the directly where the `/NC` folder is installed; the `$NCPath` name should not end with `/NC`.

EDIT THE FOLLOWING PATH STRINGS:

```
In[ ]:= $NCPath = "/Users/jam99/Dropbox";  
$UniDynPath =  
    "/Users/jam99/Dropbox/MarohnGroup__Software_Library/UniDyn/  
    unidyn";
```

YOU SHOULD NOT NEED TO EDIT ANYTHING FROM HERE ONWARDS.

Load the package

Append the package path to the system path. Before trying to load the package, ask *Mathematica* to find it. This is a test that we directed *Mathematica* to the correct directory. The output of this command should be the full system path to the `UniDyn.m` file.

```
In[ ]:= $Path = AppendTo[$Path, $NCPath];  
$Path = AppendTo[$Path, $UniDynPath];  
FindFile["UniDyn`"]  
FindFile["NC`"]
```

```
Out[ ]:= /Users/jam99/Dropbox/MarohnGroup__Software_Library/UniDyn/unidyn/UniDyn.m
```

```
Out[ ]:= /Users/jam99/Dropbox/NC/init.m
```

Now that we are confident that the path is set correctly, load the package. Setting the global `$VerboseLoad` variable to `True` will print out the help strings for key commands in the package.

```
In[ ]:= $VerboseLoad = True;
Needs["UniDyn`"]
```

NC: You are using the version of NCAIgebra which is found in: "/Users/jam99/Dropbox/NC/".

Join: Incompatible elements in $\text{Join}\left[\int \text{intt} \rightarrow \text{RowBox}\left[\left\{\int, \text{RowBox}\left[\{\blacksquare, \text{RowBox}\left[\{d, \square\}\}\right]\right\}\right], \right.\right.$
 $\text{dintt} \rightarrow \text{RowBox}\left[\left\{\text{SubsuperscriptBox}\left[\int, \blacksquare, \square\right], \text{RowBox}\left[\{\square, \text{RowBox}\left[\{d, \square\}\}\right]\right\}\right],$
 $\text{rintt} \rightarrow \text{RowBox}\left[\left\{\text{UnderscriptBox}\left[\int, \text{RowBox}\left[\{\blacksquare, \in, \square\}\right], \square\right\}\right], \text{sumt} \rightarrow \text{RowBox}\left[\left\{\text{UnderoverscriptBox}\left[\right.\right.\right.$
 $\left.\left.\sum, \text{RowBox}\left[\{\blacksquare, =, \square\}\right], \square\right\}\right], \ll 40 \gg, \text{cK} \rightarrow \text{TemplateBox}\left[\{\}, \text{CombinatorK}\right], \text{cS} \rightarrow \text{TemplateBox}\left[\{\}, \right.$
 $\left.\text{CombinatorS}\right], \text{cW} \rightarrow \text{TemplateBox}\left[\{\}, \text{CombinatorW}\right], \text{cY} \rightarrow \text{TemplateBox}\left[\{\}, \right.$
 $\left.\text{CombinatorY}\right]\left|\right.\rangle, \ll 9 \gg, \ll 3 \gg\right]$ cannot be joined.

Join: Incompatible elements in $\text{Join}\left[\int \text{intt} \rightarrow \text{RowBox}\left[\left\{\int, \text{RowBox}\left[\{\blacksquare, \text{RowBox}\left[\{d, \square\}\}\right]\right\}\right], \right.\right.$
 $\text{dintt} \rightarrow \text{RowBox}\left[\left\{\text{SubsuperscriptBox}\left[\int, \blacksquare, \square\right], \text{RowBox}\left[\{\square, \text{RowBox}\left[\{d, \square\}\}\right]\right\}\right],$
 $\text{rintt} \rightarrow \text{RowBox}\left[\left\{\text{UnderscriptBox}\left[\int, \text{RowBox}\left[\{\blacksquare, \in, \square\}\right], \square\right\}\right], \text{sumt} \rightarrow \text{RowBox}\left[\left\{\text{UnderoverscriptBox}\left[\right.\right.\right.$
 $\left.\left.\sum, \text{RowBox}\left[\{\blacksquare, =, \square\}\right], \square\right\}\right], \ll 40 \gg, \text{cK} \rightarrow \text{TemplateBox}\left[\{\}, \text{CombinatorK}\right], \text{cS} \rightarrow \text{TemplateBox}\left[\{\}, \right.$
 $\left.\text{CombinatorS}\right], \text{cW} \rightarrow \text{TemplateBox}\left[\{\}, \text{CombinatorW}\right], \text{cY} \rightarrow \text{TemplateBox}\left[\{\}, \right.$
 $\left.\text{CombinatorY}\right]\left|\right.\rangle, \ll 9 \gg, \ll 4 \gg\right]$ cannot be joined.

 NCAlgebra - Version 5.0.6
 Compatible with Mathematica Version 10 and above

Authors:

J. William Helton*
 Mauricio de Oliveira&

* Math, UCSD, La Jolla, CA
 & MAE, UCSD, La Jolla, CA

with major earlier contributions by:

Mark Stankus\$
 Robert L. Miller‡

\$ Math, Cal Poly San Luis Obispo
 ‡ General Atomics Corp

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 Helton and Miller June 1991
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The program was written by the authors and by:

David Hurst, Daniel Lamm, Orlando Merino, Robert Obar,
 Henry Pfister, Mike Walker, John Wavrik, Lois Yu,
 J. Camino, J. Griffin, J. O'vall, T. Shaheen, John Shopple.
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For NCAlgebra updates see:

www.github.com/NCAlgebra/NC
www.math.ucsd.edu/~ncalg

 .. NCAlgebra: All lower cap single letter symbols (e.g. a,b,c,...) were set as noncommutative.

.. CreateOperator: CreateOperator[] is used to batch-define a bunch of operators. Example: CreateOperator[{{lx,
 ly, lz},{Sx,Sy,Sz}}] will create six operators; each of the operators in the first list is meant to commute with
 each of the operators in the second list.

- ... **CreateScalar**: `CreateScalar[list]` is used to batch-define a bunch of scalars. The parameter `list` can be a single scalar or a list of scalars. Example: `CreateScalar[{w1,w2}]`.
- ... **NCSort**: `NCSort[list]` sorts the operators in `list` into canonical order.
- ... **SortedMult**: `SortedMult[list]` returns `Mult[list$ordered]`, where `list$ordered` are the elements of `list` sorted into canonical order.
- ... **MultSort**: `MultSort[NonCommutativeMultiply[list]]` returns `NonCommutativeMultiply[list$ordered]`, where `list$ordered` are the elements of `list` sorted into canonical order.
- ... **Comm**: `Comm[a,b]` calculates the commutator of two operators.
- ... **SpinSingle\$CreateOperators**: `SpinSingle$CreateOperators[lx,ly,lz,L]` creates l_x , l_y , and l_z angular momentum operators and defines their commutation relations. When the total angular momentum $L = 1/2$, additional rules are defined to simplify products of the angular momentum operators. When the total angular momentum L is unspecified, no such simplification rules are defined.
- ... **OscSingle\$CreateOperators**: `OscSingle$CreateOperators[aL,aR]` creates a raising operator a_R and a lowering operator a_L for single harmonic oscillator and defines the operator commutation relations.
- ... **Evolve**: `Evolve[H, t, ρ]` represents unitary evolution of the density operator ρ for a time t under the Hamiltonian H . This function expands according to simplification rules but leaves the evolution unevaluated.
- ... **Evolver**: `Evolver[H, t, $\rho(0)$]` calculates $\rho(t) = \text{Exp}[-i H t] \rho(0) \text{Exp}[+i H t]$, assuming that H is time independent, according to the commutation rules followed by $\rho(0)$ and H .

Execute the units tests in batch

Included with the package are a number of files, ending in “-tests.m”, that contain tests of the package’s functions -- so-called unit tests. Set the working directory to the package directory and pretty-print the directory name.

```
In[ ]:= SetDirectory[$UniDynPath];
```

```
TableForm[{{$UniDynPath}}, TableHeadings -> {None, {"Directory"}}]
```

Out[]//TableForm=

```
Directory
```

```
/Users/jam99/Dropbox/MarohnGroup__Software_Library/UniDyn/unidyn
```

Get the names of all the unit-testing files included with the package (following my convention that the unit testing file end in “-tests.m”). Pretty-print the names of the unit-test files included with the package.

```
In[ ]:= fn = FileNames["*-tests.m"];
TableForm[{{fn}}, TableHeadings → {None, {"Test files found"}}]
```

Out[]//TableForm=

```
Test files found
Comm-tests.m
Evolve-tests.m
Mult-tests.m
OpCreate-tests.m
Osc-tests.m
Spins-tests.m
```

Finally, carry out the unit tests.

```
In[ ]:= tr = TestReport /@ fn;
TableForm[Table[tr [[k]], {k, 1, Length[tr]}]]
```

Out[]//TableForm=

TestReportObject [		Title: Test Report: Comm-tests.m Success rate: 100% Tests run: 12]
TestReportObject [		Title: Test Report: Evolve-tests.m Success rate: 100% Tests run: 27]
TestReportObject [		Title: Test Report: Mult-tests.m Success rate: 100% Tests run: 20]
TestReportObject [		Title: Test Report: OpCreate-tests.m Success rate: 100% Tests run: 23]
TestReportObject [		Title: Test Report: Osc-tests.m Success rate: 100% Tests run: 20]
TestReportObject [		Title: Test Report: Spins-tests.m Success rate: 100% Tests run: 14]

Make a report.

```
In[158]:= tests$passed$total =
  Plus @@ (tr[[#]]["TestsSucceededCount"] & /@ List @@ Table[k, {k, 1, Length[tr]}]);
tests$failed$total = Plus @@
  (tr[[#]]["TestsFailedCount"] & /@ List @@ Table[k, {k, 1, Length[tr]}]);
Print[Style[ToString[tests$passed$total] <> " tests passed",
  FontWeight → Bold, FontSize → 18, FontColor → Blue]];
Print[Style[ToString[tests$failed$total] <> " tests failed",
  FontWeight → Bold, FontSize → 18, FontColor → Red]]
```

116 tests passed

0 tests failed

Execute the units tests one-by-one

Re-execute the tests in an order determined by us. This is useful for debugging. Running the *Evolve-test.m* file takes a minute.

```
In[ ]:= SetDirectory[ $UniDynPath ];
TableForm[ { { $UniDynPath } }, TableHeadings -> { None, { "Directory" } } ]
```

```
Out[ ]:= TableForm=
Directory
/Users/jam99/Dropbox/MarohnGroup__Software_Library/UniDyn/unidyn
```

```
In[ ]:= $VerboseLoad = False;
Needs["UniDyn`"]
```

```
In[ ]:= TestReport[FileNames["OpCreate-tests.m"]][[1]]
```

```
Out[ ]:= TestReportObject[
+ ✓ Title: Test Report: OpCreate-tests.m
Success rate: 100% Tests run: 23
]
```

```
In[ ]:= TestReport[FileNames["Mult-tests.m"]][[1]]
```

```
Out[ ]:= TestReportObject[
+ ✓ Title: Test Report: Mult-tests.m
Success rate: 100% Tests run: 20
]
```

```
In[ ]:= TestReport[FileNames["Comm-tests.m"]][[1]]
```

```
Out[ ]:= TestReportObject[
+ ✓ Title: Test Report: Comm-tests.m
Success rate: 100% Tests run: 12
]
```

```
In[ ]:= TestReport[FileNames["Spins-tests.m"]][[1]]
```

```
Out[ ]:= TestReportObject[
+ ✓ Title: Test Report: Spins-tests.m
Success rate: 100% Tests run: 14
]
```

```
In[ ]:= TestReport[FileNames["Evolve-tests.m"]][[1]]
```

```
Out[ ]:= TestReportObject[
+ ✓ Title: Test Report: Evolve-tests.m
Success rate: 100% Tests run: 27
]
```

Congratulations

At this point you should have

(1) loaded the NCAIgebra and UniDyn packages and

(2) run the UniDyn units tests demonstrating that UniDyn is working as expected.