DINO Manual Addendum
0.8.0 to 0.8.4

1 Shell

Only commands issued interactively, ie not from a shell script, are written into the logfile, and only if they did not produce an error.

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Upon exit, the current orientation (scene property `rtc`, see below) is written into the logfile.

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Commands from shell scripts are no longer added to the history.

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Three new RPN stack operators:

dist expects two coordinates on the stack, calculates the distance between them

angle expects three coordinates (ABC) on the stack, calculates the angle between $\overline{AB}$ and $\overline{BC}$

torsion expects four coordinates on the stack, calculates the torsion angle defined by them

2 Scene and GUI

Scene commands `hide` and `show` globally turn display of objects off or on. Useful for running large script files, e.g.

beginning of script
`scene hide`
all commands follow, executed faster since objects not displayed
...
at end of script
```
.*.* hide // optionally turn all objects off
scene show
```

•

Scene property `rtc` stores the current rotation, transation and centering in one matrix, e.g.

```
echo [scene get rtc]
scene set rtc= ...
```

•

`$CS` saves a unique atom number (as `.struct:#NUM`).

•

Upon picking, `$CP` is set to the position of the picked atom.

•

On linux: A spaceball under the control of the joystick driver is recognized.

•

Xresources applicable for the top level widget to include the preferred depth (`applicationDepth`), visualid (`visualID`) or visual class (`visualClass`); e.g. add

```
dino*applicationDepth:  24
```

to your `.Xdefaults` file to get 24 bit color with an 8bit default root window.

3 General Dataset Stuff

Four new formats:

- ▷ CHARMM scalar field from the new ESP module, dataset type `charmmb`, extension `.cpot`
- ▷ Experimental support for ADS surface interface format, dataset type `ads`
- ▷ GRASP surface file, dataset type `grasp`, extension `.grasp`
- ▷ New BDTRJ format

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Extension `.ccp4` for CCP4 scalar field (type `ccp4` and extension `.map`).

•

Load command flag `-c`, applicable to UHBD scalar fields: will cause a conversion of the grid units based on the `scale` entry in the header, usually represents $\frac{kcal}{mol \cdot e}$ to kT conversion.

•

Datasets (structure, scalar-field and surface) may be transformed using the properties `rot` (a rotation matrix R), `trans` (a translation vector T), `rcen` (the center of rotation C) and `rtc` (a compact description of the three previous ones), as well as the commands `rotx`, `roty`, `rotyz` and `transx`, `transy`, `transz`.

$$p' = R \cdot (p - C) + C + T$$

4 Structure Dataset

The rendering state is updated automatically after a `set` command.

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The property `rad` determines the thickness of tube rendering on a per residue basis.

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Atoms with x>=9999 are ignored upon reading.

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New mode `single` and new parameter `-delay` for trajectory command `play`.

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Nucleic Acids

The spline function will pass through the phosphate atoms for rendering modes `tube` and `sline`, but through the `C3'` atom of the sugar unit for rendering mode `hsc`.

Properties `color1`, `color2` and `color3` are used to change color of NA backbone, sugar and base, respectively. Property `color` applies to all three (and overrides the individual ones).

Render property `sugart` and `baset` can be used to set the thickness of sugar and base cartoon.

Nucleic acid residues in coordinate files are identified by their residue names as `A`, `C`, `T`, `G`, `U` or `ADE`, `CYT`, `GUA`, `THY`, `URI`.

5 Surface Dataset

Upon loading a surface dataset, the flag `-rn` will cause a renormalization of the normal vectors (usually not necessary).

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Clipped surface objects can be rendered solid with

```
dino> .surf.obj render solid,solidc=COLOR
```

and turned hollow again with

```
dino> .surf.obj render !solid
```

It is important to note that the far clipping plane must be completely behind the surface for this feature to work properly. This technique uses the stencil buffer, and hence may be *really* slow on OpenGL implementations that have no hardware accelerated stencil buffer.

6 Scalar Field Dataset

Scalar field contour level defaults to 1.0s for types `ccp4`, `xplora`, `xplorb`, `cnsa` and `cnsb`, for all others to 0.0.

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A new scalar-field object type `slab` has been introduced. It is defined by a plane, described by a center (property `center`) and direction (property `dir`), and displays the minimal rectangle defined by the intersection of this plane with the scalar-field grid volume.

This rectangle is subdivided into $n \times n$ points (property `size`, must fulfill $n = 2^a$, $2 < a < 9$), which may be colored according to the scalar-field grid values they intersects with.

Example:

```
dino> .ds new -type slab -name s -set center={0,0,0},dir={0,0,1},size=128
dino> .ds.s set color=green:yellow -range val=-0.3:0.7
```

•

Scalar-field dataset properties `vm` and `vc` can be used to change the grid values according to

$$v_{new} = v_{old} \cdot vm + vc$$

The default values are $vm = 1.0$ and $vc = 0.0$.

7 Topograph Dataset

The render properties `polyf` and `polyu` change the polygon offset for object type `surface`.

•

An asymmetric image may be loaded now.

8 Geom Dataset

The default object color can be set with

```
dino> .geom.obj set color=COLOR
```

•

The render mode `tube` will first generate a spline through consecutive object points, and then render the spline as a tube of radius `rad`.

9 Export

Raster Images

TIFF output flagged as deprecated. Please use only PNG.

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Normally, the raster image is prepared in an offscreen rendering context. The write flag `-dump` will circumvent this by using the pixels directly from the on-screen window. It is important to note that the gfx window should not be obstructed by any other window.

POVray

POVray output has been pretty much rewritten from scratch! For more detail, please see the new POVray tutorial on the homepage.