NAME

ecx - library for electrochemistry

SYNOPSIS

```
ecx (Fortran): use ecx
ecx (C): include "ecx.h"
ecx (python): import pyecx
```

DESCRIPTION

ecx a Fortran library for providing a collection of routines for electrochemistry. A C API allows usage from C, or can be used as a basis for other wrappers. A Python wrapper allows easy usage from Python.

It covers:

o kinetics
Nernst, Butler-Volmer

o electrochemical
Impedance, Admittance, Circuit Elements, Equivalent Circuits

o photoelectrochemistry
Photocurrent, Band-gap, space charge.

The C API is defined by adding a prefix to the functions from the Fortran API due to the lack of module/namespace feature in the C language. The functions are therefore following this template: (c_prefix)fortran_func.

- (ecx_)get_version
- (ecx_core_)kTe
- (ecx_eis_)z
- mm
- (ecx_kinetics_)nernst
- (ecx_kinetics_)sbv
- (ecx_kinetics_)bv
- (ecx_eis_)z

NOTES

To use ecx within your fpm <https://github.com/fortran-lang/fpm> project, add the following lines to your file:

```
[dependencies]
ecx = { git="https://github.com/MilanSkocic/ecx.git" }
```

EXAMPLE

Example in Fortran:

```
program example_in_f
    use iso_fortran_env
    use ecx
    implicit none

    real(real64) :: w(3) = [1.0d0, 1.0d0, 100.0d0]
    real(real64) :: r = 100.0d0
    real(real64) :: p(3) = 0.0d0
    character(len=1) :: e
    integer :: errstat
    complex(real64) :: zout(3)
```

```
    character(len=:), pointer :: errmsg

    p(1) = r
    e = "R"
    call z(p, w, zout, e, errstat, errmsg)
    print *, zout
    print *, errstat, errmsg
end program
```

Example in C:

```
int main(void){
    int errstat, i;
    double w[3] = {1.0, 1.0, 1.0};
    double p[3] = {100.00, 0.0, 0.0};
    ecx_cdouble z[3] = {ecx_cbuild(0.0,0.0),
                        ecx_cbuild(0.0, 0.0),
                        ecx_cbuild(0.0, 0.0)};
    char *errmsg;

    ecx_eis_z(p, w, z, 'R', 3, 3, &errstat, &errmsg);

    for(i=0; i<3;i++){
        printf("%f %f 0, creal(z[i]), cimag(z[i]));
    }
    printf("%d %s0, errstat, errmsg);
    return EXIT_SUCCESS;
}
```

Example in Python:

```
import numpy as np
import pyecx
import matplotlib.pyplot as plt

R = 100
C = 1e-6
w = np.logspace(6, -3, 100)

p = np.asarray([R, 0.0, 0.0])
zr = np.asarray(pyecx.z("R", w, p))
p = np.asarray([C, 0.0, 0.0])
zc = np.asarray(pyecx.z("C", w, p))
zrc = zr*zc / (zr+zc)
print("finish")

fig = plt.figure()
ax = fig.add_subplot(111)

ax.set_aspect("equal")
ax.plot(zrc.real, zrc.imag, "g.", label="R/C")

ax.invert_yaxis()

plt.show()
```

SEE ALSO

complex(7), **gsl**(3), **catanh**(3), **gnuplot**(1), **ecx_get_version**(3)