

# *a tutorial on inq*



Xavier Andrade, A. Correa and T. Ogitsu  
Lawrence Livermore National Laboratory  
xavier@llnl.gov

*we tricked you into thinking you  
were going to learn to use an  
electronic structure program  
today...*

*you are going to write your own*

# *History of inq*

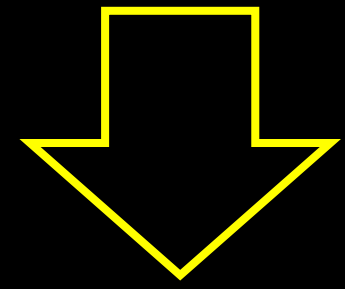
Project started  
one year ago

Objective: real-time TDDFT  
on GPUs

Use modern C++ coding  
techniques

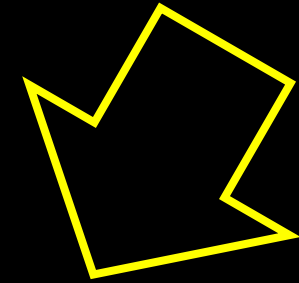
inq is a library

Users

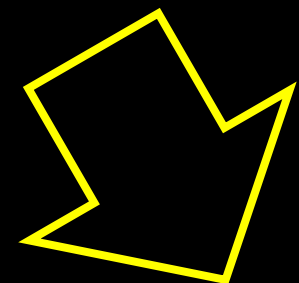
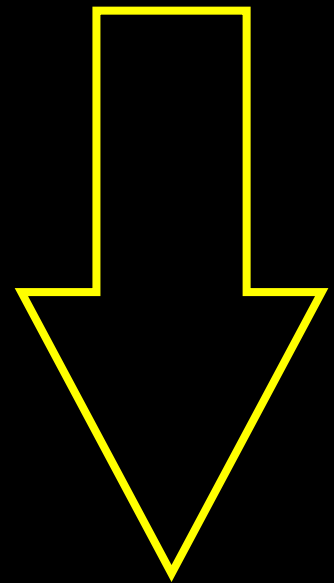


QBall

Users



QBall  
(interface under development)



inq

# *Features*

Clean design from scratch:  
13k lines of code

Designed to run on  
GPU supercomputers

Plane-wave and  
pseudopotentials

Modular and extensible  
implementation

# *Distribution*

Free software  
LGPL3 license

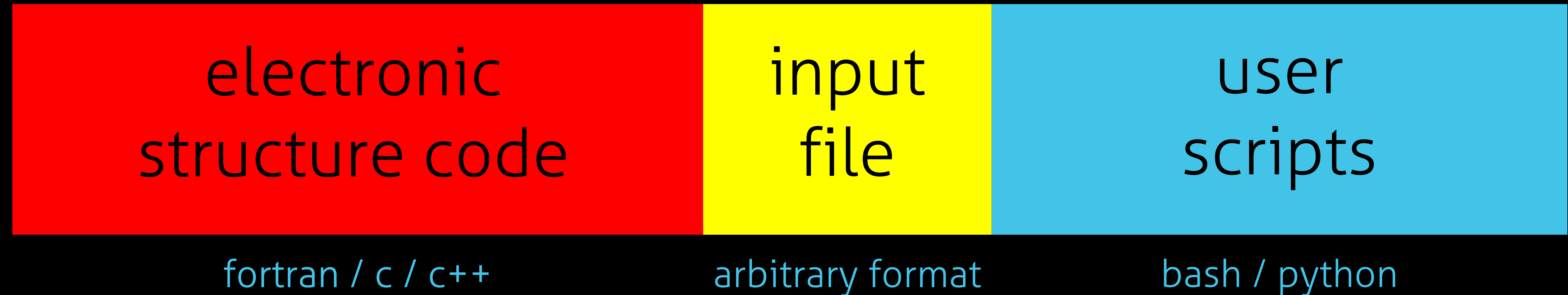
Available now from  
<http://gitlab.com/npneq/inq>

Under heavy development

# *traditional paradigm*

developers

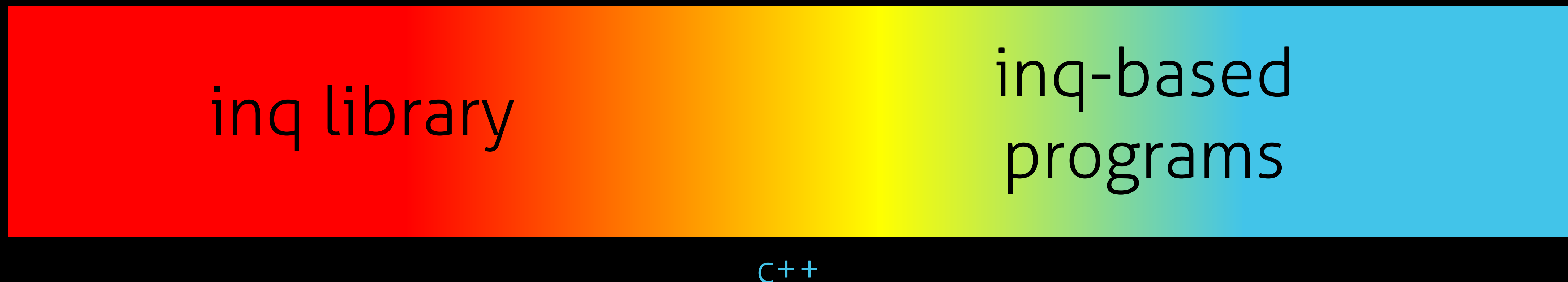
users



# *inq paradigm*

developers

users





# *Example of an inq "input file"*

```
double distance = 2.0;
```

```
vector<atom> geo;  
geo.push_back( "N" | vec3d(0.0, 0.0, -distance/2.0));  
geo.push_back( "N" | vec3d(0.0, 0.0, distance/2.0));
```

```
cell super = cell::cubic(3.0, 3.0, 6.0) | cell::periodic();
```

```
systems::ions ions(super, geo);
```

```
systems::electrons electrons(ions, basis::cutoff_energy(30.0));
```

```
auto result = ground_state::calculate(ions, electrons,  
                                       interaction::dft(),  
                                       scf::conjugate_gradient() | scf::mixing(0.1));
```

# *Compiling an inq code*

To make compilation easy we provide `inc++`, a compiler wrapper that passes all the options and libraries required

```
inc++ nitrogen.cpp -o nitrogen
```

# *Conclusions*

Not your standard electronic  
structure code

Use one language,  
not three

Work in progress, many  
features missing

Suggestions and  
contributions are welcome

# *Today's exercises*

Exercise 0: load inq in your terminal

Exercise 1: calculate a potential energy surface and  
optimize a geometry

Exercise 2: calculate a new observable

Tutorial location:

<https://gitlab.com/npneq/inq/-/wikis/Tutorial>