C++/Boost::Python programming Example with Yade-DEM

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On debian/ubuntu and connected to internet?

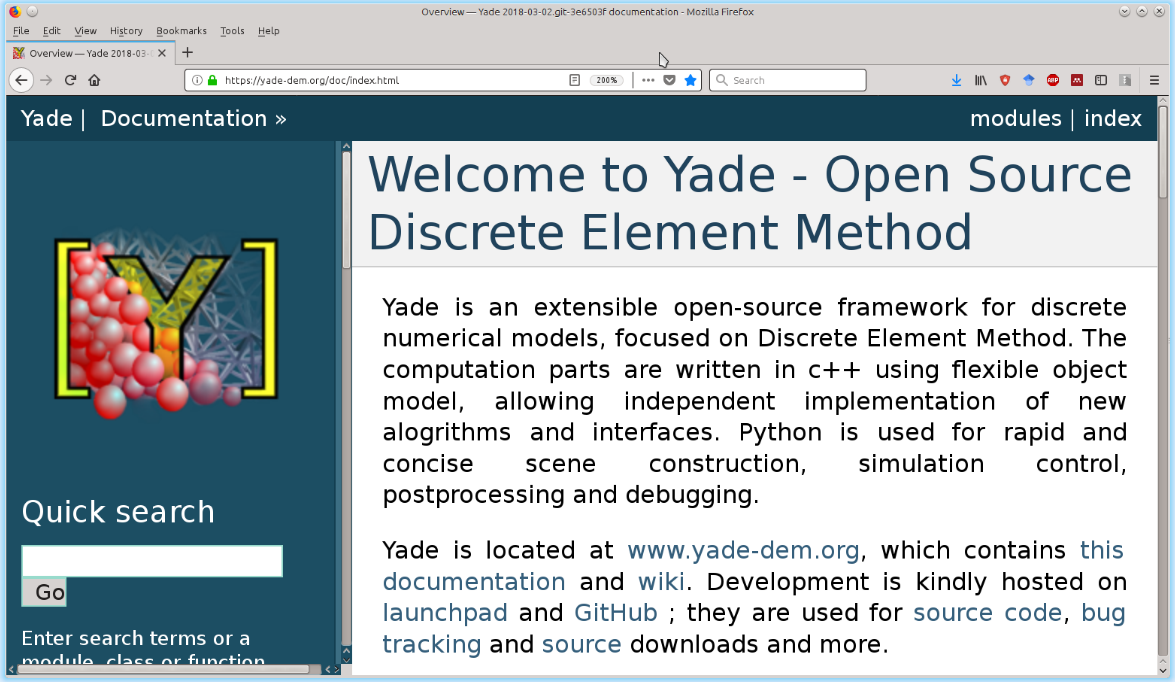
```
$ sudo apt-get install yade (~70MB)
$ yade
```

You can reproduce the example in a minute

Yade-DEM.org

- Open platform for the simulation of mechanical systems (DEM)
- Started[*] and hosted[**] at lab. 3SR / GitHub
- Developed natively on Debian/Ubuntu systems
- Compiles on CentOS, Red Hat, MS Windows (yes!),...
- Deployed on various servers (incl. Gricad/Froggy, Amazon EC,...)
- Pre-compiled packages available for Debian/Ubuntu (>2011)

[*] by Frédéric Donzé (2006)
[**] thanks to Rémi Cailletaud



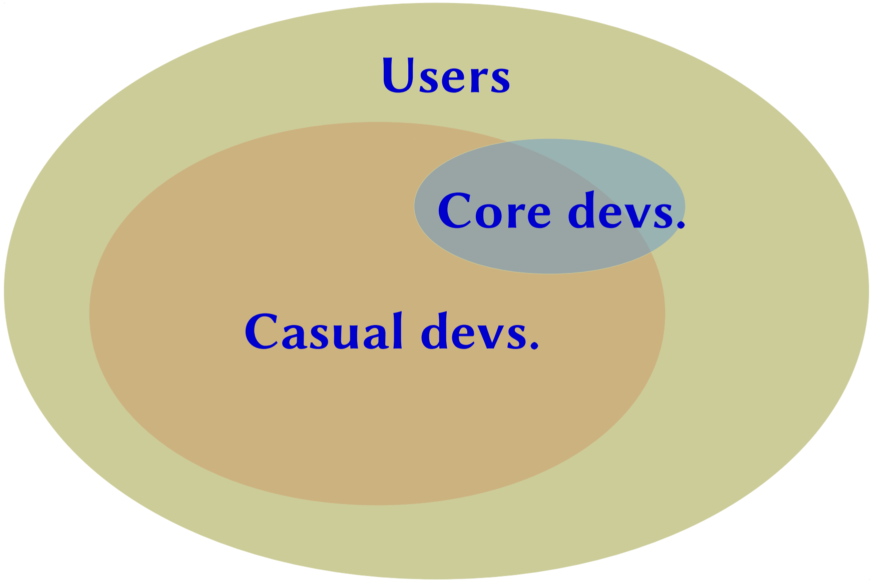
Overview — Yade 2018-03-02.git-3e6503f documentation - Mozilla Firefox

Welcome to Yade - Open Source Discrete Element Method

Yade is an extensible open-source framework for discrete numerical models, focused on Discrete Element Method. The computation parts are written in c++ using flexible object model, allowing independent implementation of new alogrithms and interfaces. Python is used for rapid and concise scene construction, simulation control, postprocessing and debugging.

Yade is located at www.yade-dem.org, which contains this documentation and wiki. Development is kindly hosted on launchpad and GitHub ; they are used for source code, bug tracking and source downloads and more.

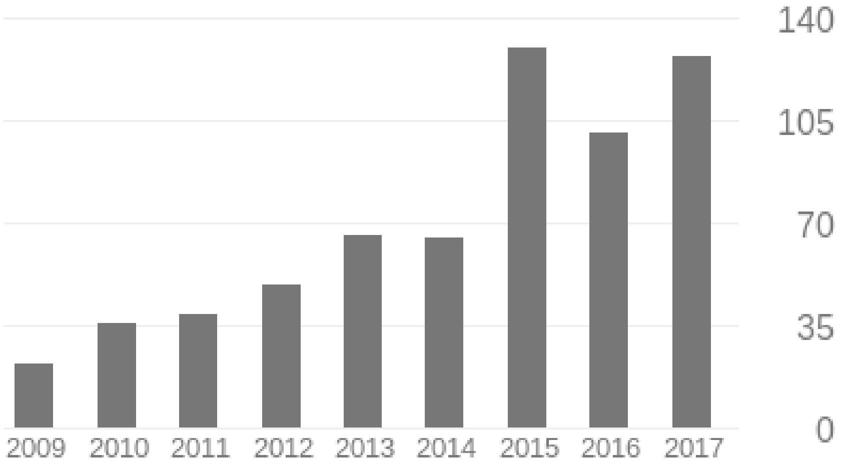
Yade-DEM.org community



Users (>100/year)

- applications in mechanics, physics, process/chemical/civil engineering…
- typically little to no time/experience for advanced programming

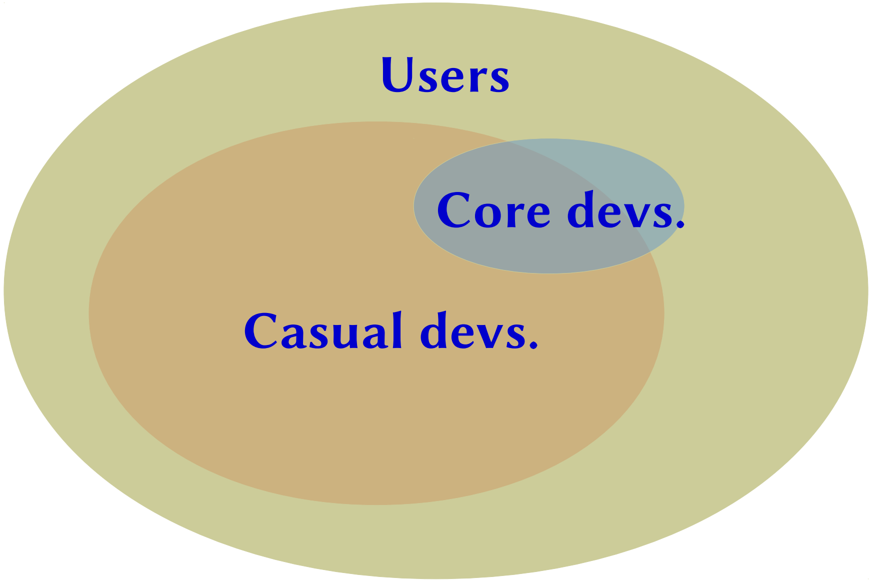
Google Scholar citations

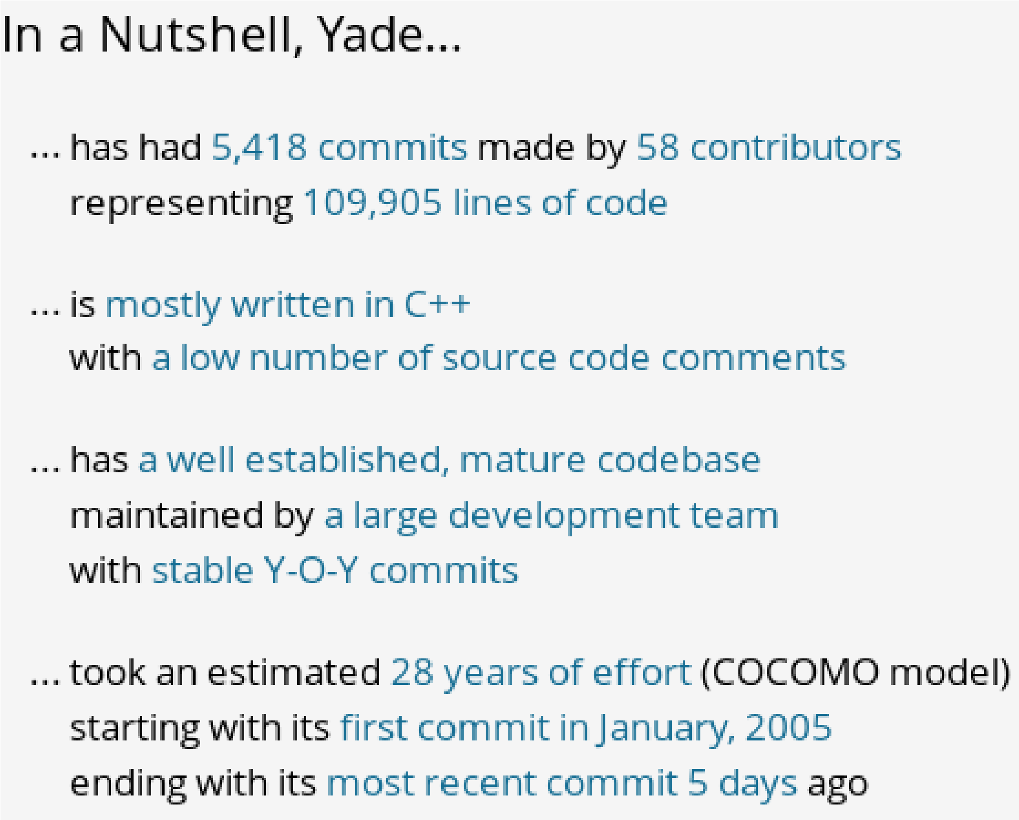


V. Šmilauer et al. (2015), **Yade Documentation 2nd ed.**
DOI 10.5281/zenodo.34073

Yade-DEM.org community

Developpers (~15/year, ~50 from begining)





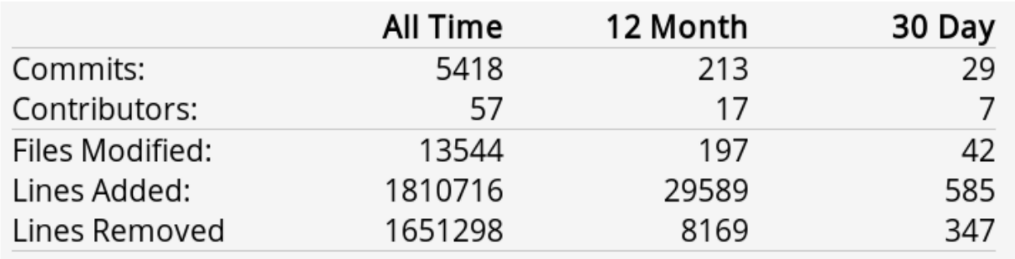
In a Nutshell, Yade...

... has had 5,418 commits made by 58 contributors representing 109,905 lines of code

... is mostly written in C++ with a low number of source code comments

... has a well established, mature codebase maintained by a large development team with stable Y-O-Y commits

... took an estimated 28 years of effort (COCOMO model) starting with its first commit in January, 2005 ending with its most recent commit 5 days ago

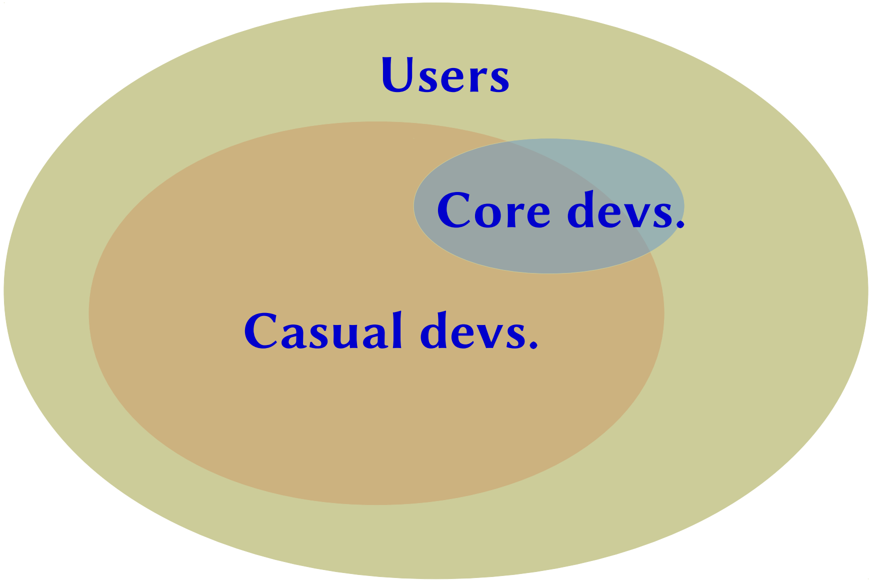


	All Time	12 Month	30 Day
Commits:	5418	213	29
Contributors:	57	17	7
Files Modified:	13544	197	42
Lines Added:	1810716	29589	585
Lines Removed	1651298	8169	347

Stats from OpenHub.net

Yade-DEM.org community

Developpers (~10/year, ~40 from begining)

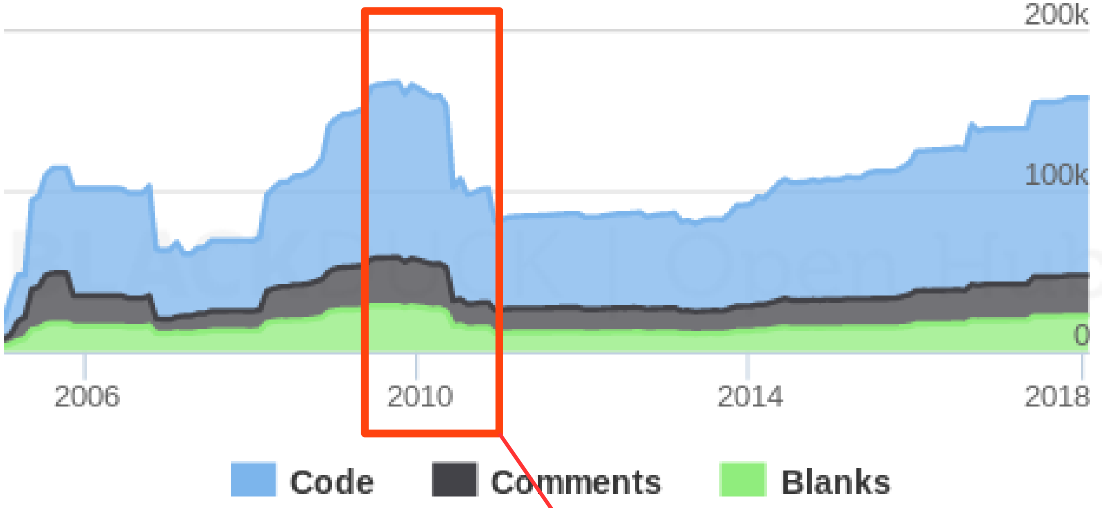


Users

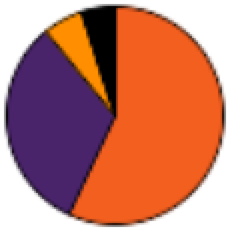
Core devs.

Casual devs.

Lines of Code



Languages



🟧	C++	57%	🟪	Python	32%
🟧	C	6%	⬛	7 Other	5%

Stats from GitHub.com

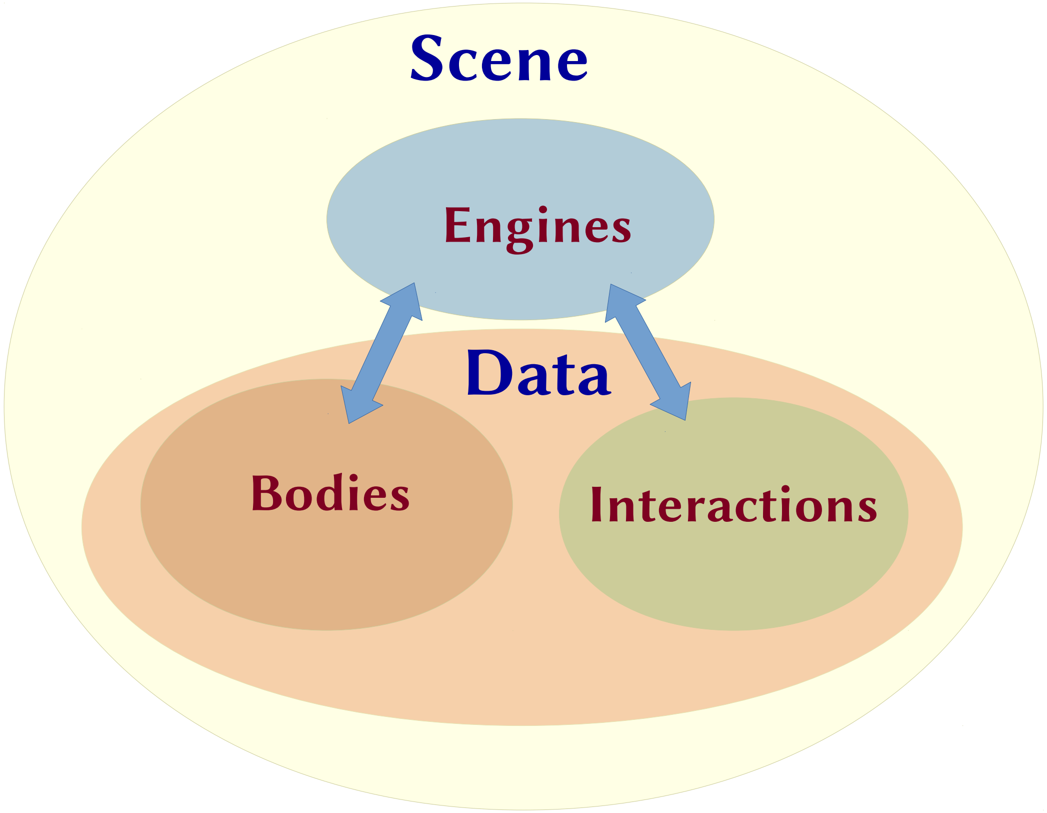
Scene & interface(s)

A "Scene" is mainly three lists (of c++ objects) with transition rules (see live example)

- **Bodies** (data)
  position
  velocity
  physical properties

- **Engines** (act once per iteration)
  laws of physics
  boundary/field conditions
  contact detection
  recorders
  …

- **Interactions** (auto-updated data)
  physical state: deformation, forces, …

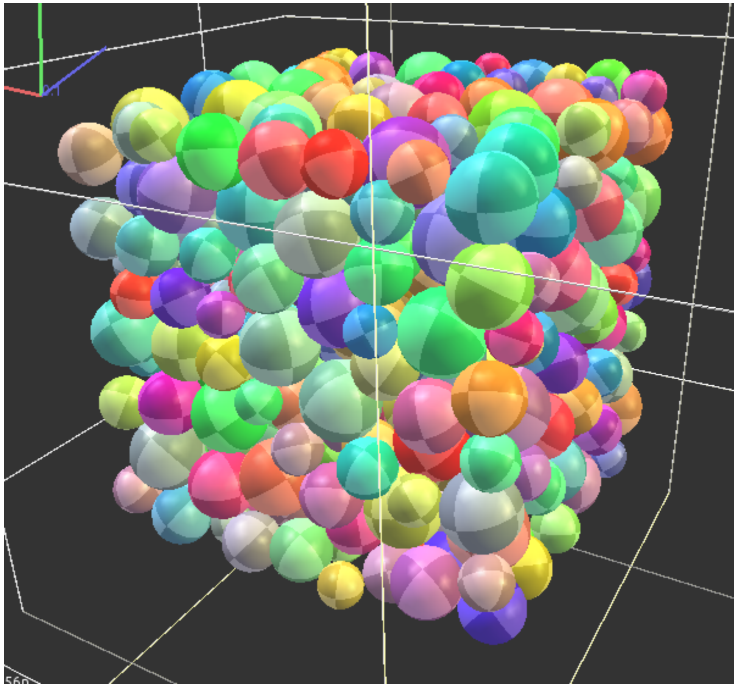


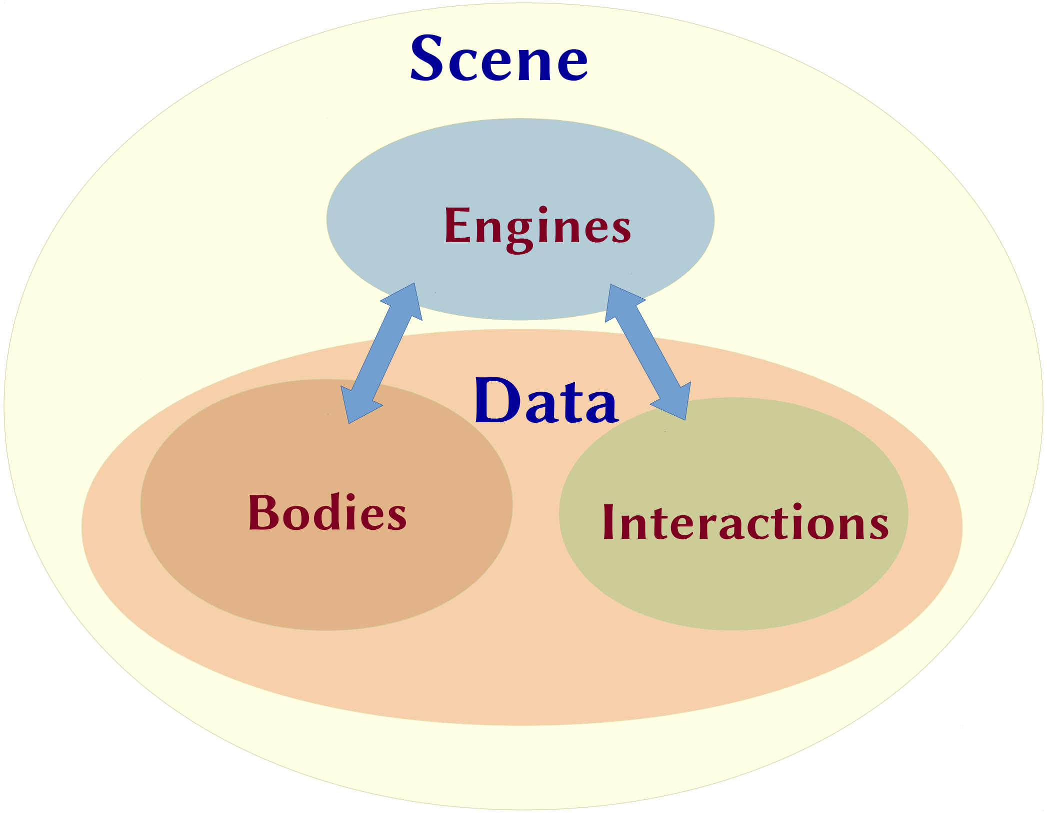
Scene & interface(s)

Interfaces to a c++ (DEM) code

1) Hard-code

change the source code + recompile,
i.e. no interface.





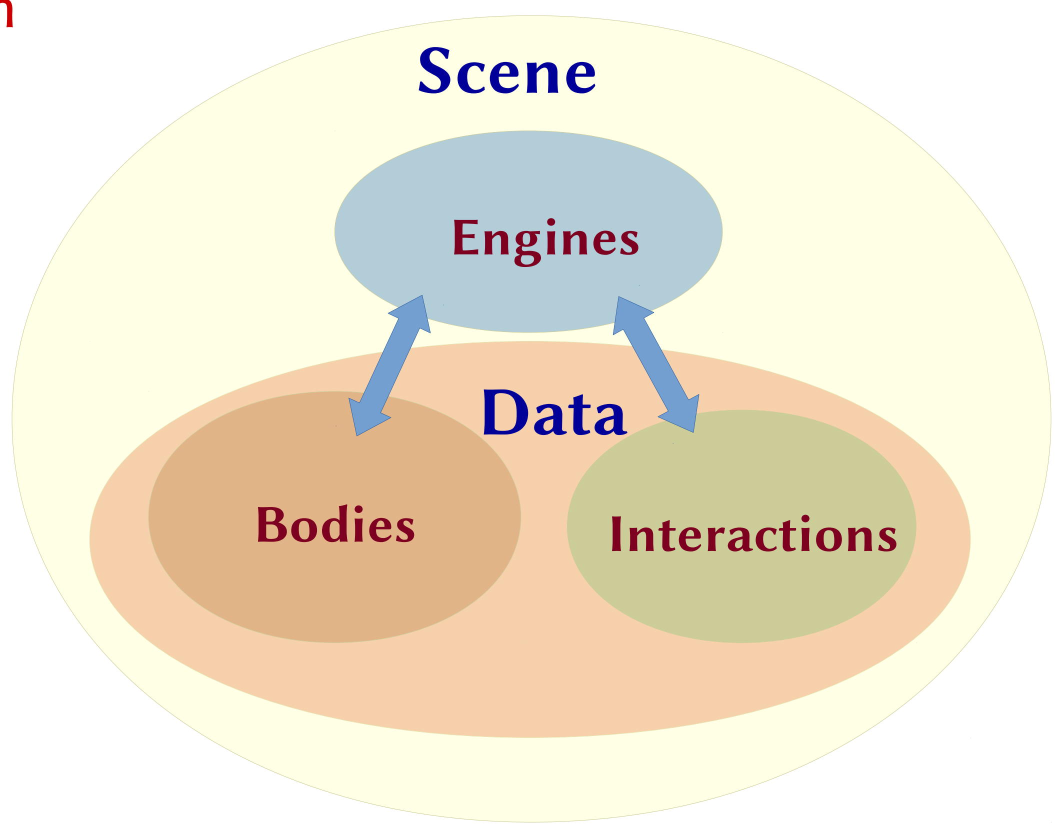
Scene & interface(s)

Interfaces to a c++ code

1) Hard-code (i.e no interface...)

⟶ maximizes flexibility, but:

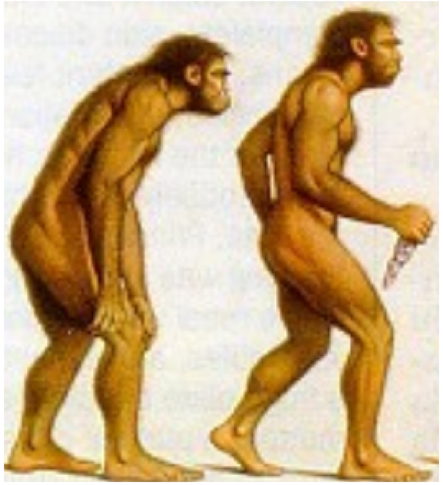
- vertical learning curve
- difficult to debug / no interactivity
- no batch execution
- tends to mix user-specific code with actual source code (dev=user...)
- smart hacks are difficult to share with others

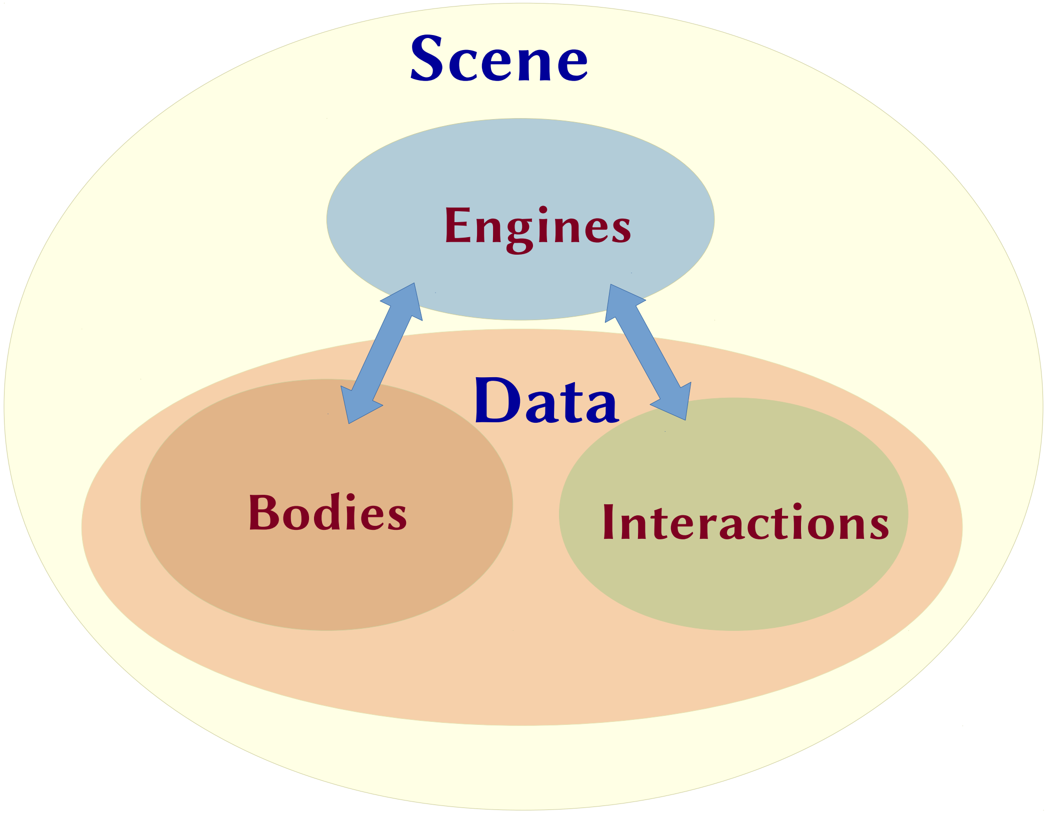


Scene & interface(s)

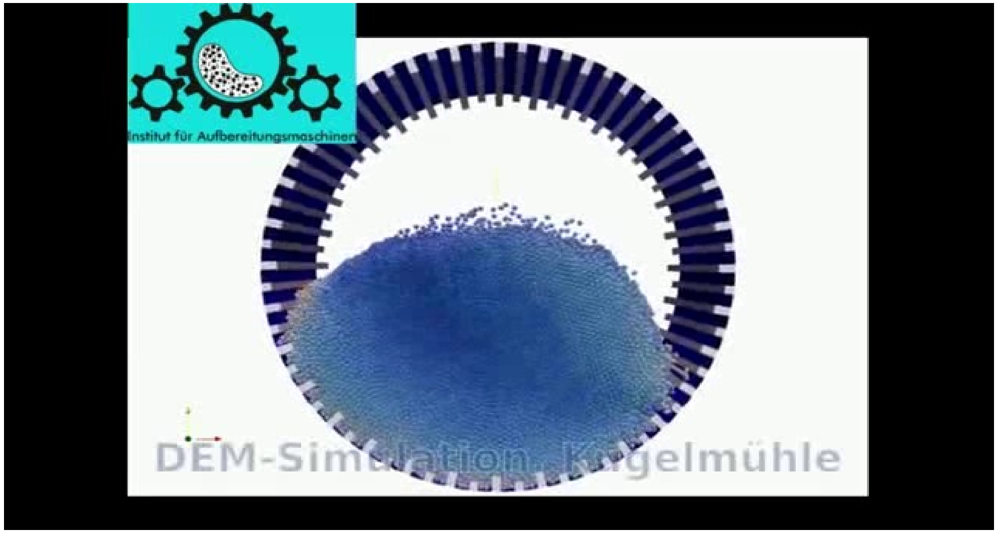
Interfaces

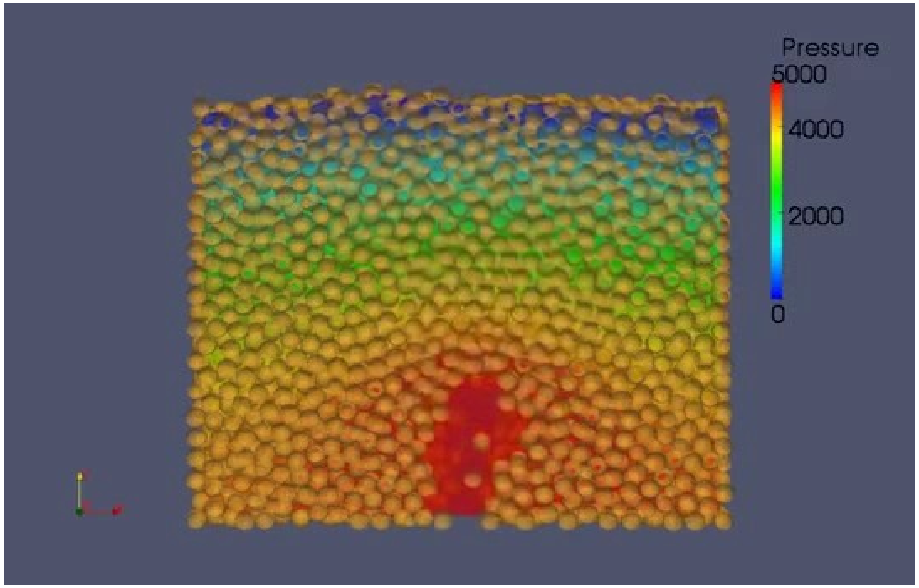
1) ~~Hardcode~~
2) Write input files
3) +Read output files

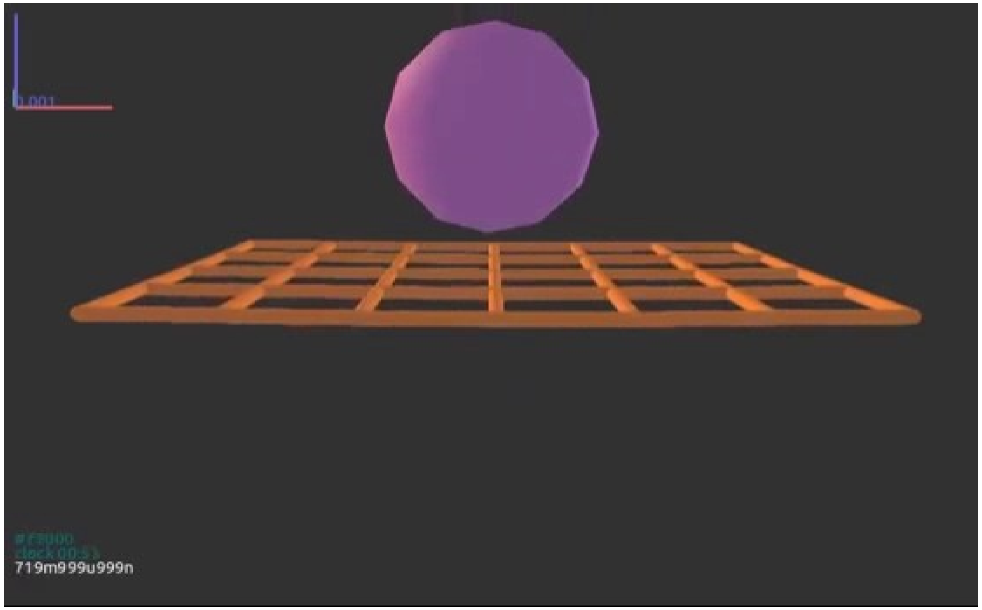


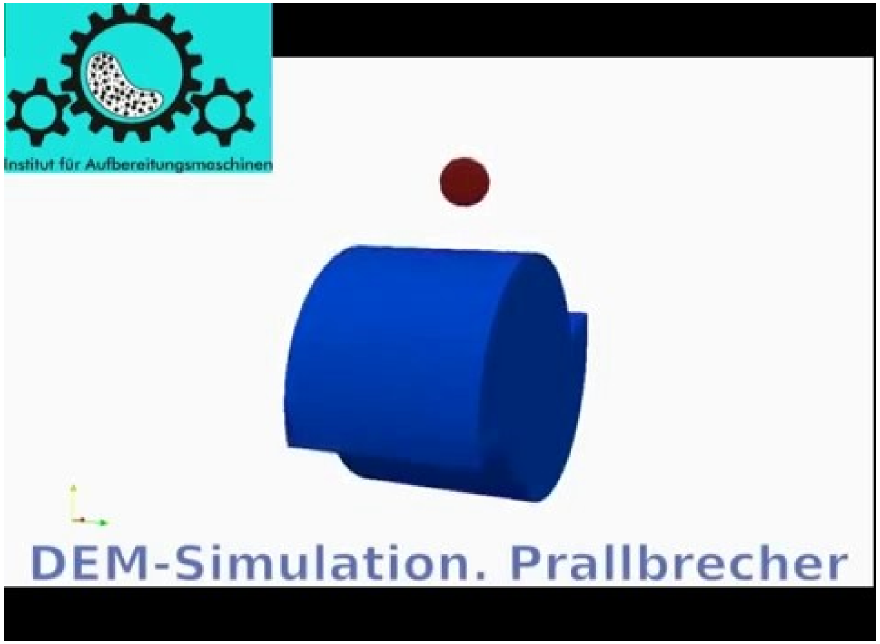


Scene & interface(s)


Institut für Aufbereitungsmaschinen
DEM-Simulation. Kugelmühle





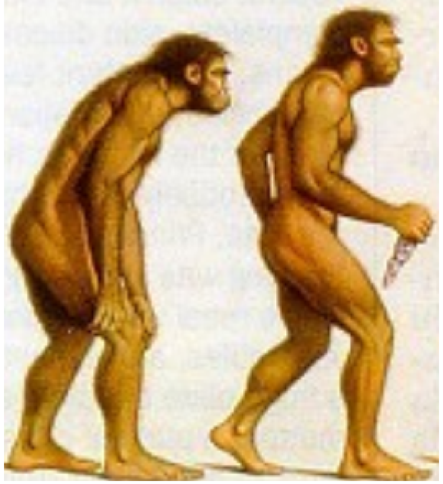

Institut für Aufbereitungsmaschinen
DEM-Simulation. Prallbrecher

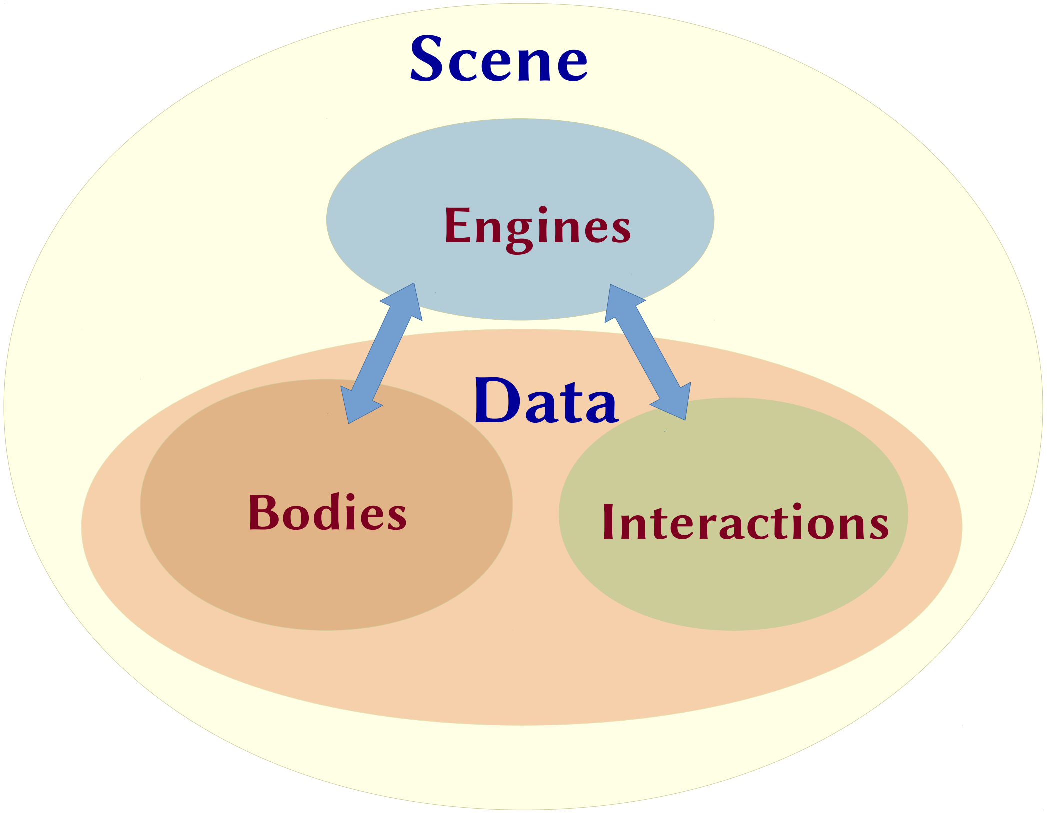
Scene & interface(s)

Interfaces

1) ~~Hardcode~~
2) Write input files
3) +Read output files

- no flexibility
- no extensibility
- no feedback loop

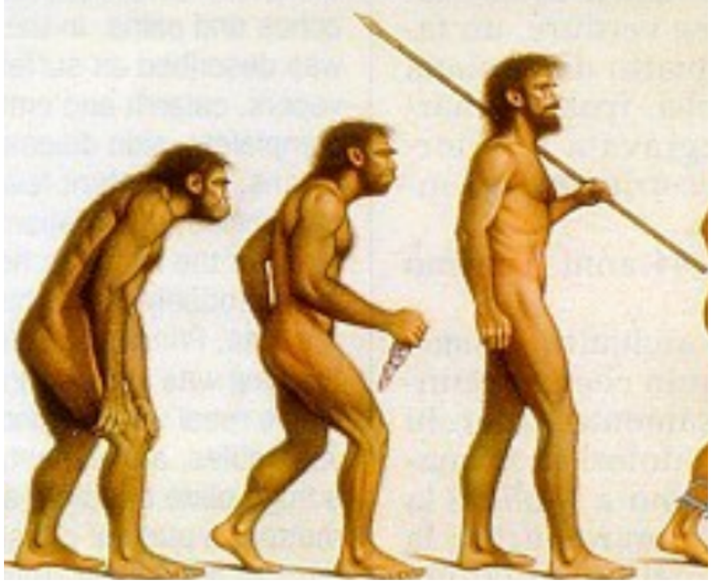




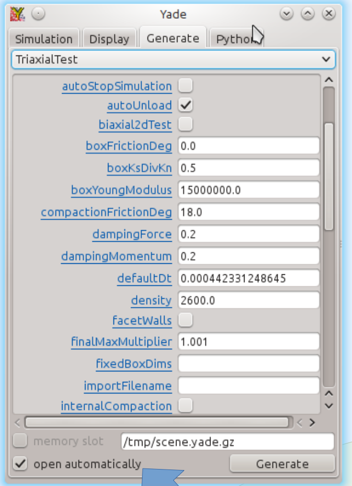
Scene & interface(s)

Interfaces

- ~~Hardcode~~
- ~~Write input files~~
- ~~Read output files~~
- Graphical user interface (GUI)



Qt Controller



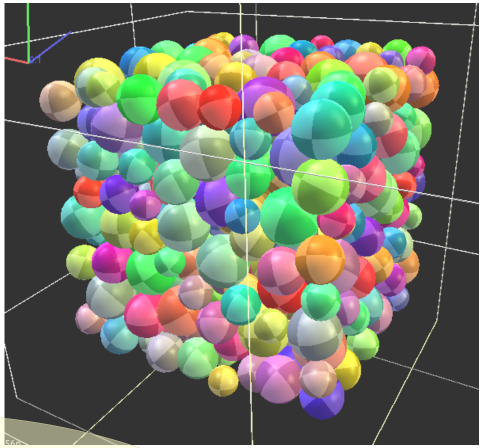
TriaxialTest

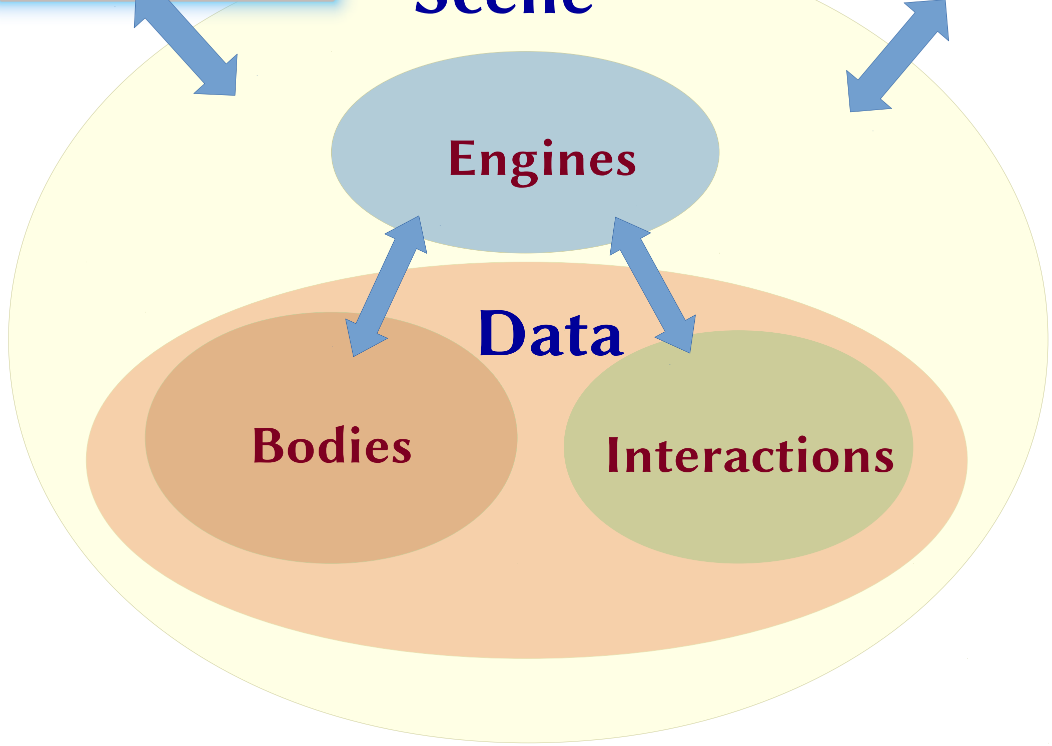
autoStopSimulation	□
autoUnload	☑
biaxial2dTest	□
boxFrictionDeg	0.0
boxKsDivKn	0.5
boxYoungModulus	15000000.0
compactionFrictionDeg	18.0
dampingForce	0.2
dampingMomentum	0.2
defaultDt	0.000442331248645
density	2600.0
facetWalls	□
finalMaxMultiplier	1.001
fixedBoxDims	
importFilename	
internalCompaction	□

□ memory slot /tmp/scene.yade.gz

☑ open automatically

QGLView



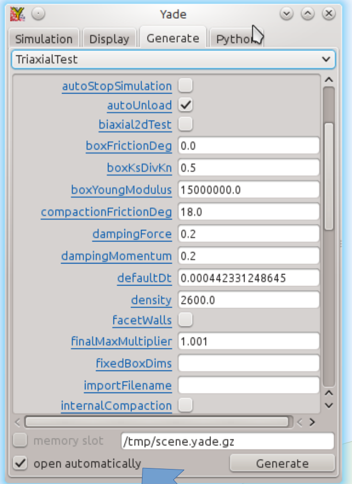


Scene & interface(s)

Interfaces

- ~~Hardcode~~
- ~~Write input files~~
- ~~Read output files~~
- Graphical user interface (GUI)

Qt Controller



Yade

Simulation | Display | Generate | Python

TriaxialTest

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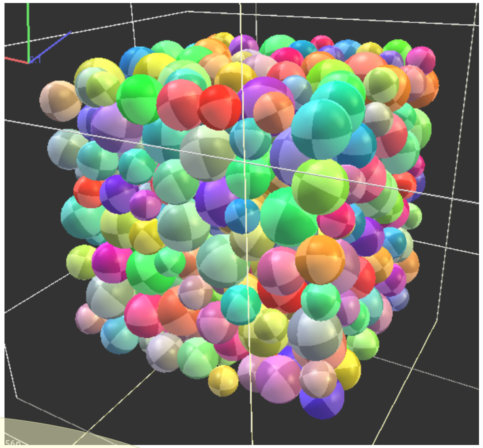
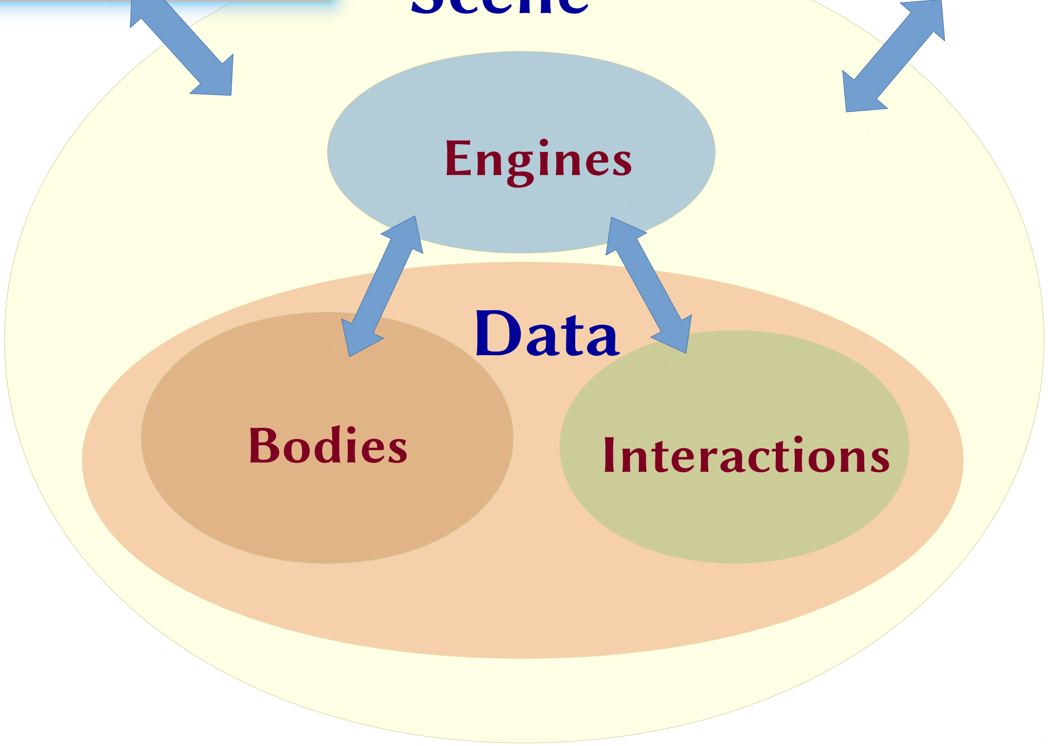
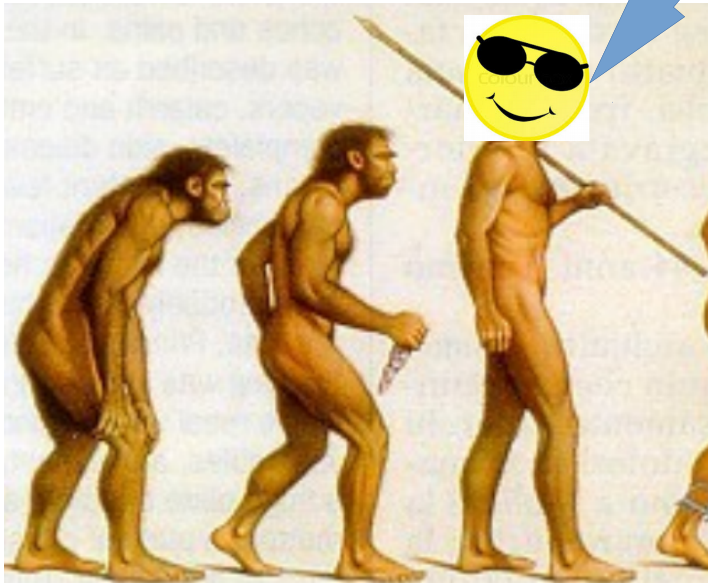
☑ open automatically

QGLView





Pride?



Scene & interface(s)

Interfaces

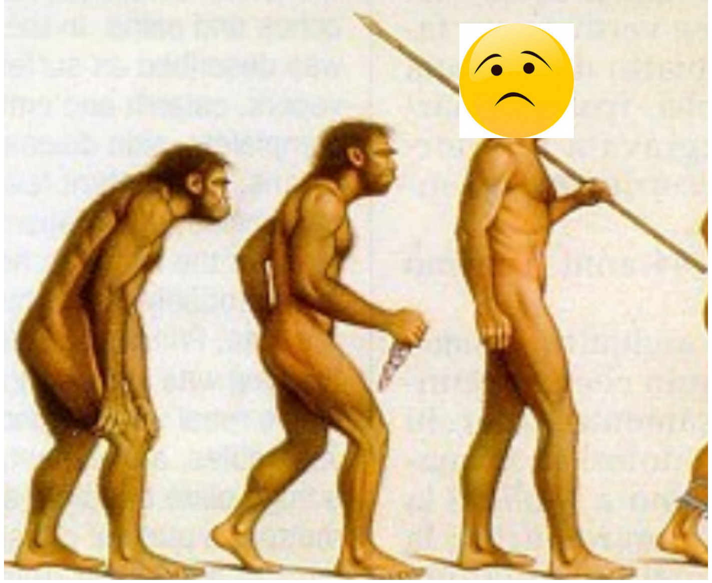
- ~~Hardcode~~
- ~~Write input files~~
- ~~Read output files~~
- Graphical user interface (GUI)

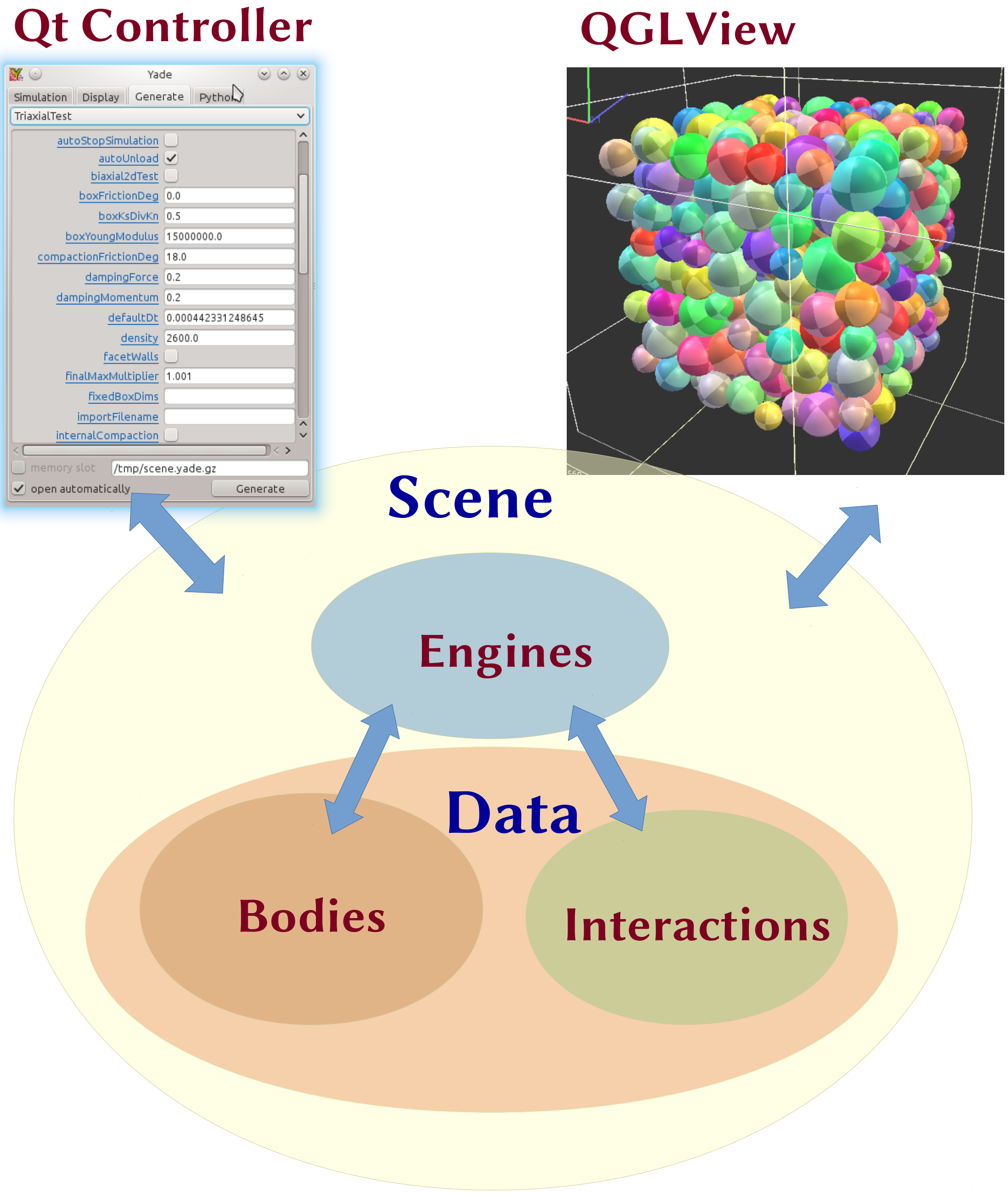
- no flexibility

- no extensibility

- no feedback loop

= I/O files + complex design





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facetWalls	□
finalMaxMultiplier	1.001
fixedBoxDims	
importFilename	
internalCompaction	□

□ memory slot /tmp/scene.yade.gz

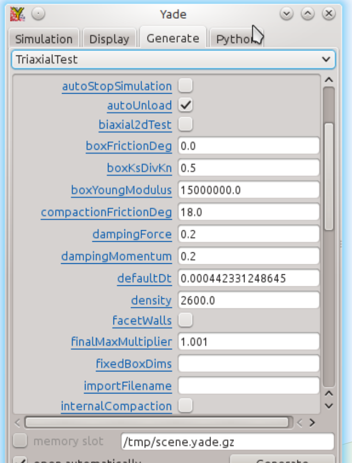
☑ open automatically

Scene & interface(s)

Interfaces

- ~~Hardcode~~
- ~~Write input files~~
- ~~Read output files~~
- ~~Graphical user interface (GUI)~~
- Command line interface (CLI)

Qt Controller



Yade

Simulation | Display | Generate | Pytho

TriaxialTest

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autoUnload ☑
biaxial2dTest □
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compactionFrictionDeg 18.0
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density 2600.0
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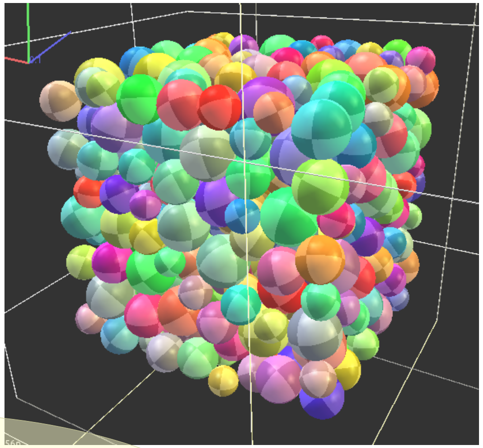
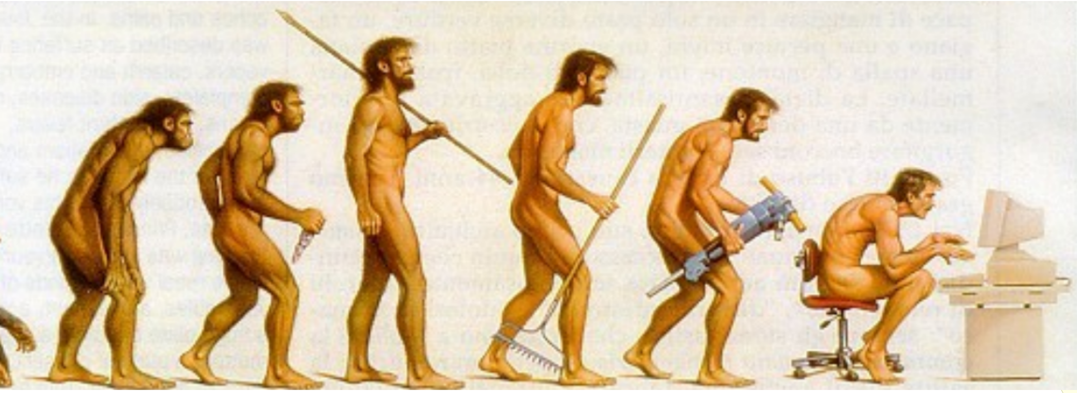
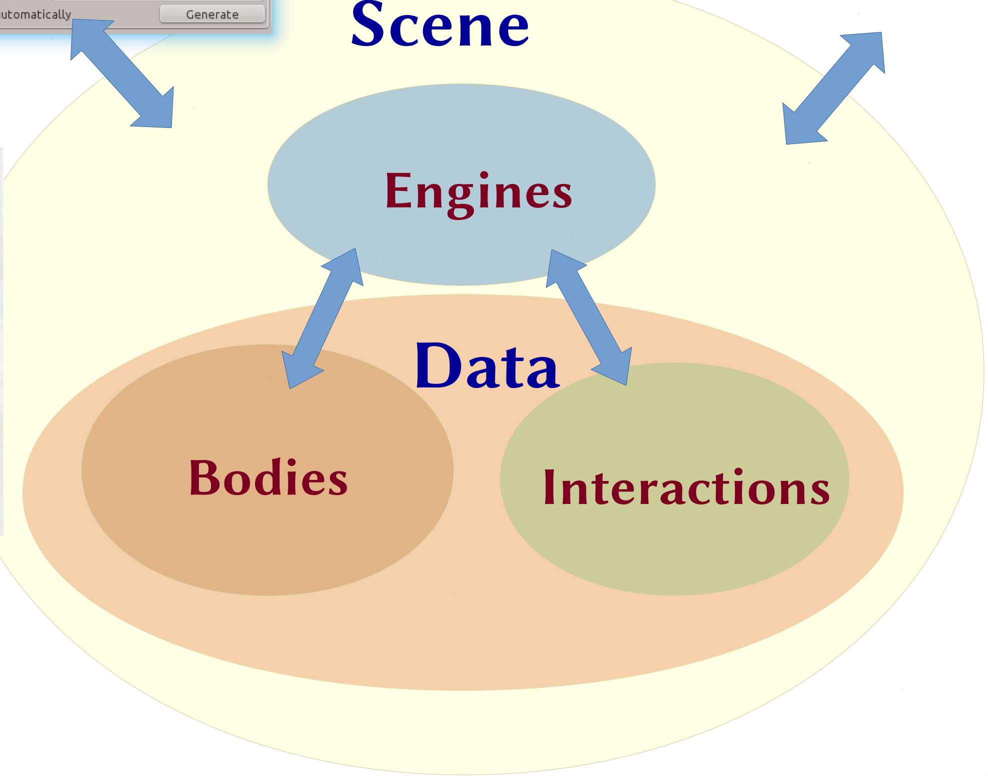
☑ open automatically Generate

QGLView







Scene & interface(s)

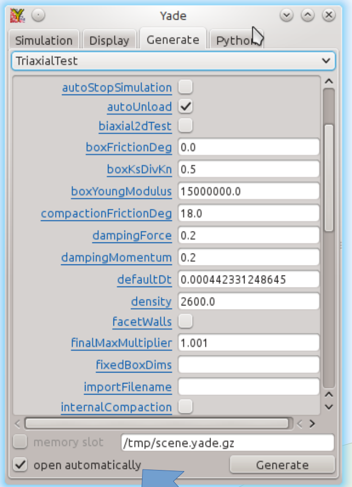
Interfaces

- Hardcode
- Write input files
- Read output files
- Graphical user interface (GUI)
- Command line interface (CLI)

State of the art in DEM softwares

- Most in-house codes stuck in the I/O files paradigm
- In the 90's Itasca© started developing the "FISH" language for their DEM softwares (coded in C++)
- ~2004 it was possible to pass arguments to FISH functions and to declare local variables...
- ~2014 Itasca© started considering Python!

Qt Controller



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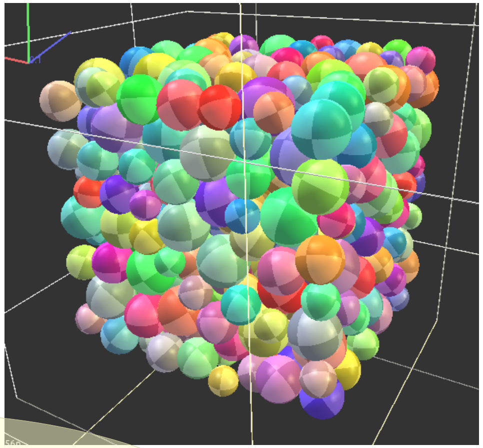
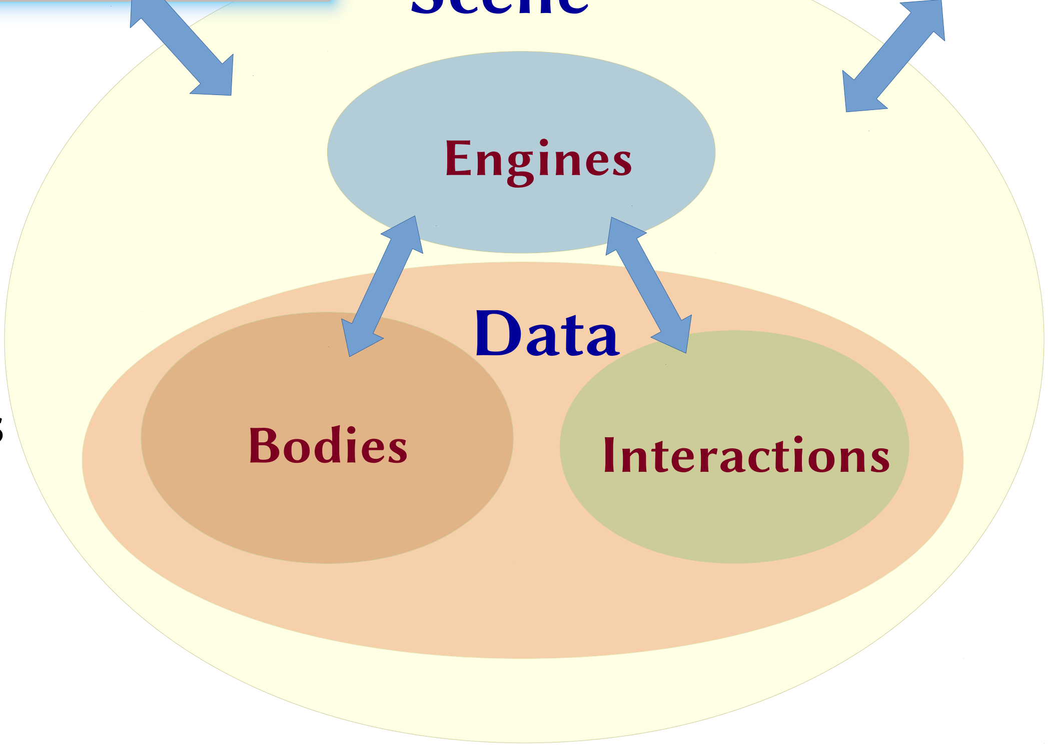
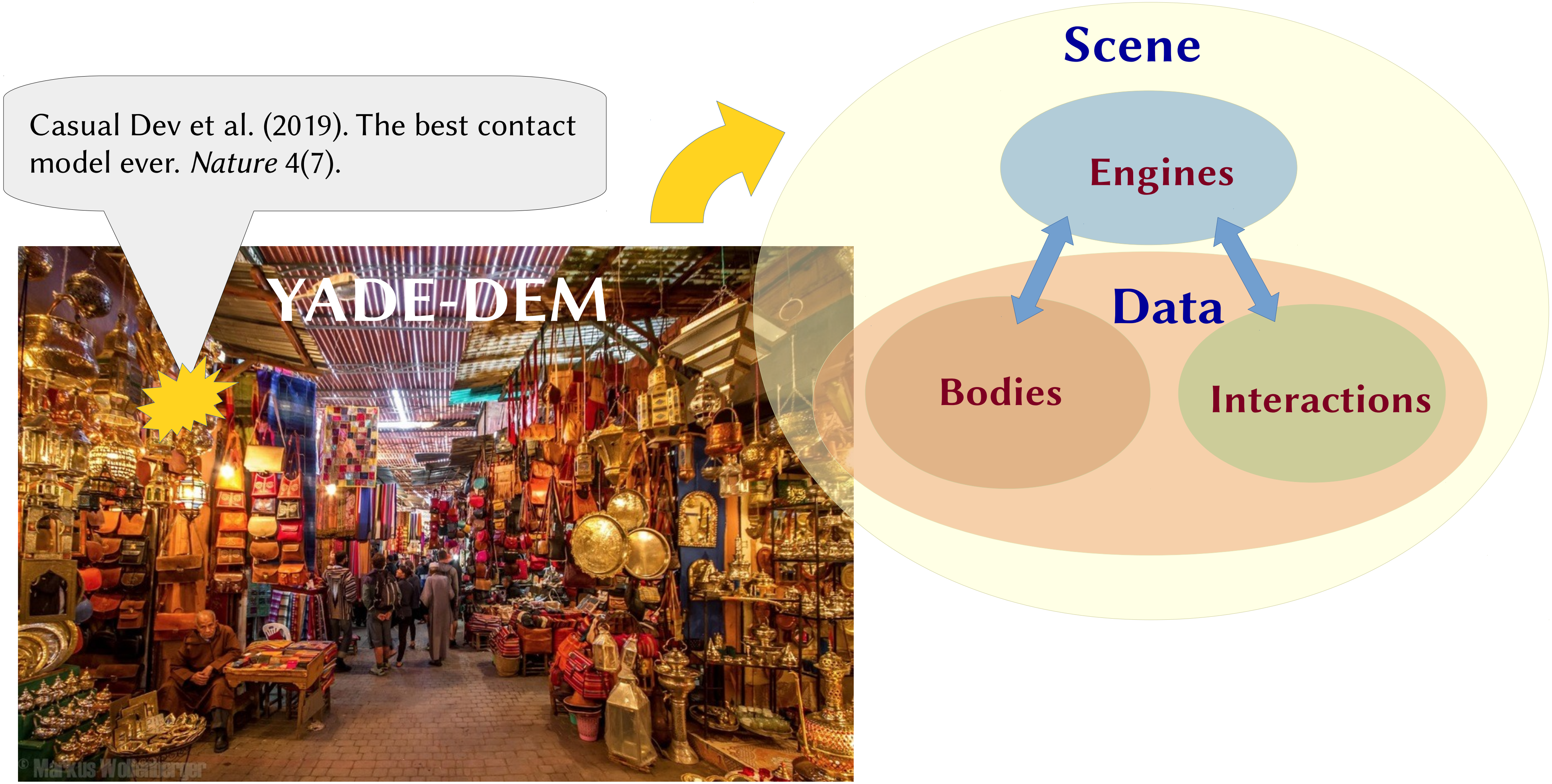




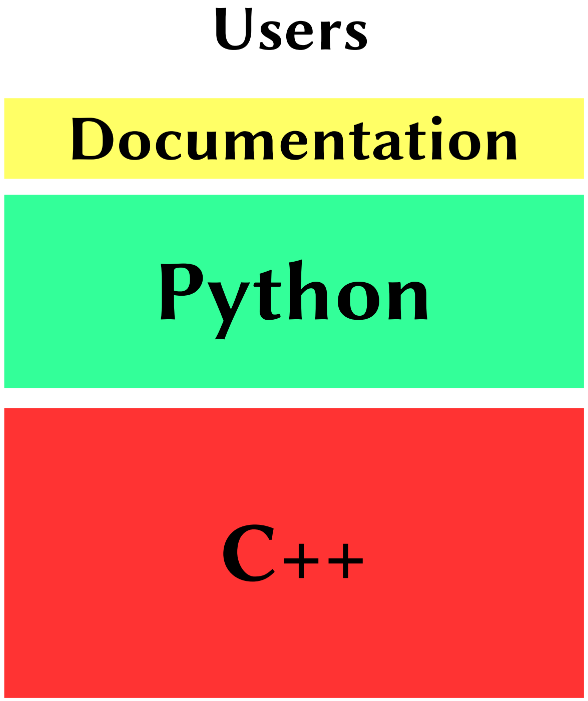
A challenging development problem:

YADE-DEM is a bazaar

Casual Dev et al. (2019). The best contact model ever. *Nature* 4(7).



A challenging development problem



Users

Documentation

Python

C++

Users

little to no time/experience in programming

Needs:

- documentation
- computational efficiency
- simplicity of usage
- flexibility
- interactivity

Casual devs.

want to implement something new (contact model, particle shape,...)

Needs:

- simplicity of implementation
- low commit barrier
- will hardly learn new programing techniques

Core devs.

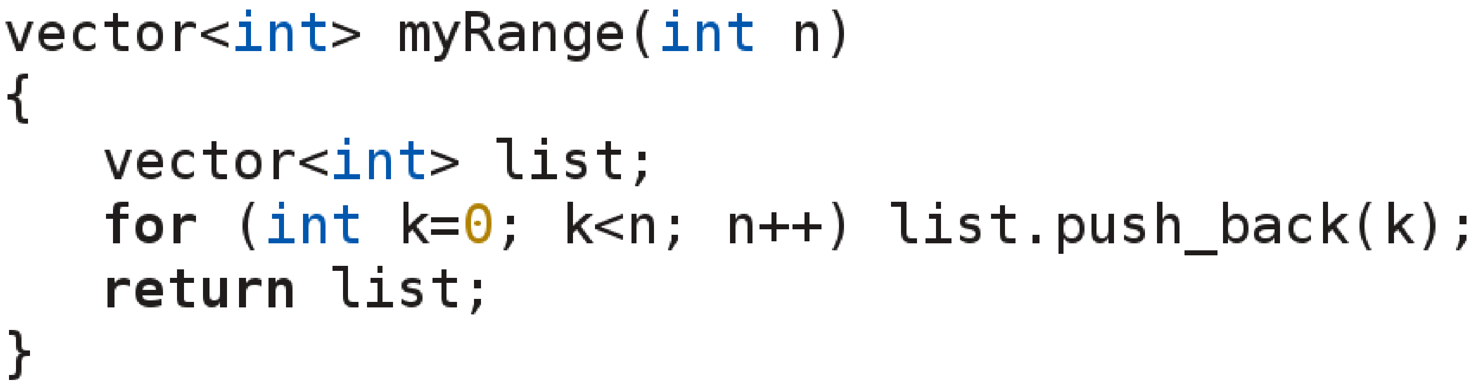
Needs:

- **minimize workload**

boost::python

Example

Consider this piece of C++ code that we want to use in python:

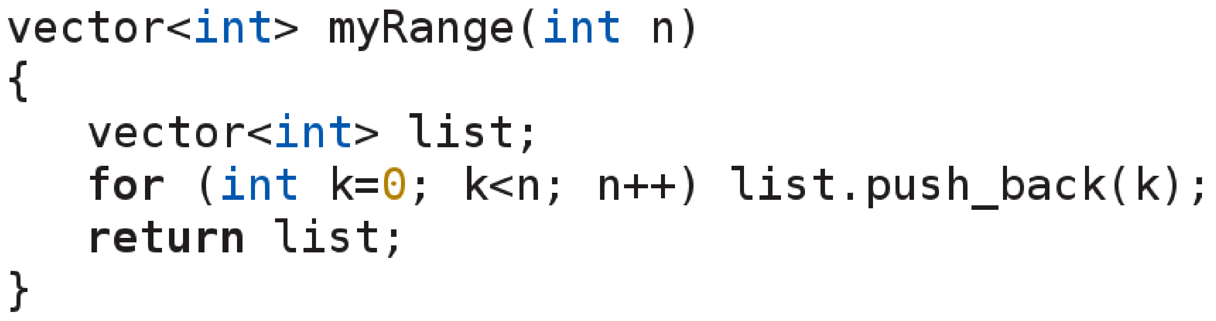


```
vector<int> myRange(int n)
{
   vector<int> list;
   for (int k=0; k<n; n++) list.push_back(k);
   return list;
}
```

boost::python

Example

Consider this piece of C++ code that we want to use in python:



```
vector<int> myRange(int n)
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}
```
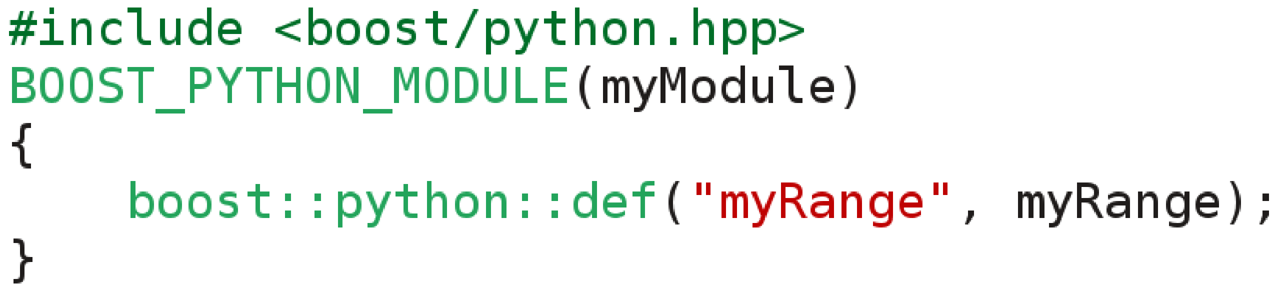
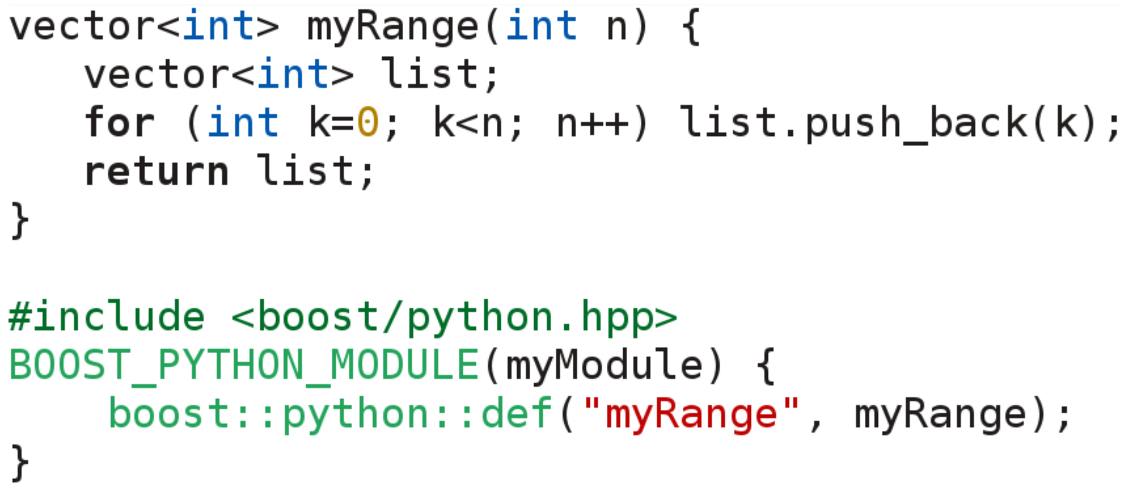

It is enough to append:



```
#include <boost/python.hpp>
BOOST_PYTHON_MODULE(myModule)
{
     boost::python::def("myRange", myRange);
}
```

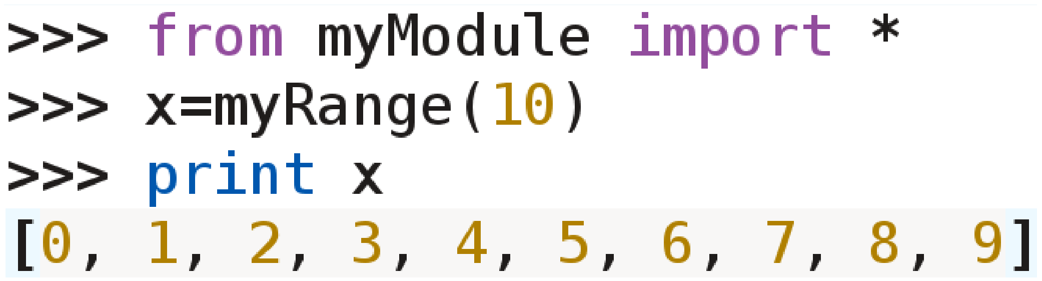
boost::python

Example



```
vector<int> myRange(int n) {
   vector<int> list;
   for (int k=0; k<n; n++) list.push_back(k);
   return list;
}

#include <boost/python.hpp>
BOOST_PYTHON_MODULE(myModule) {
    boost::python::def("myRange", myRange);
}
```

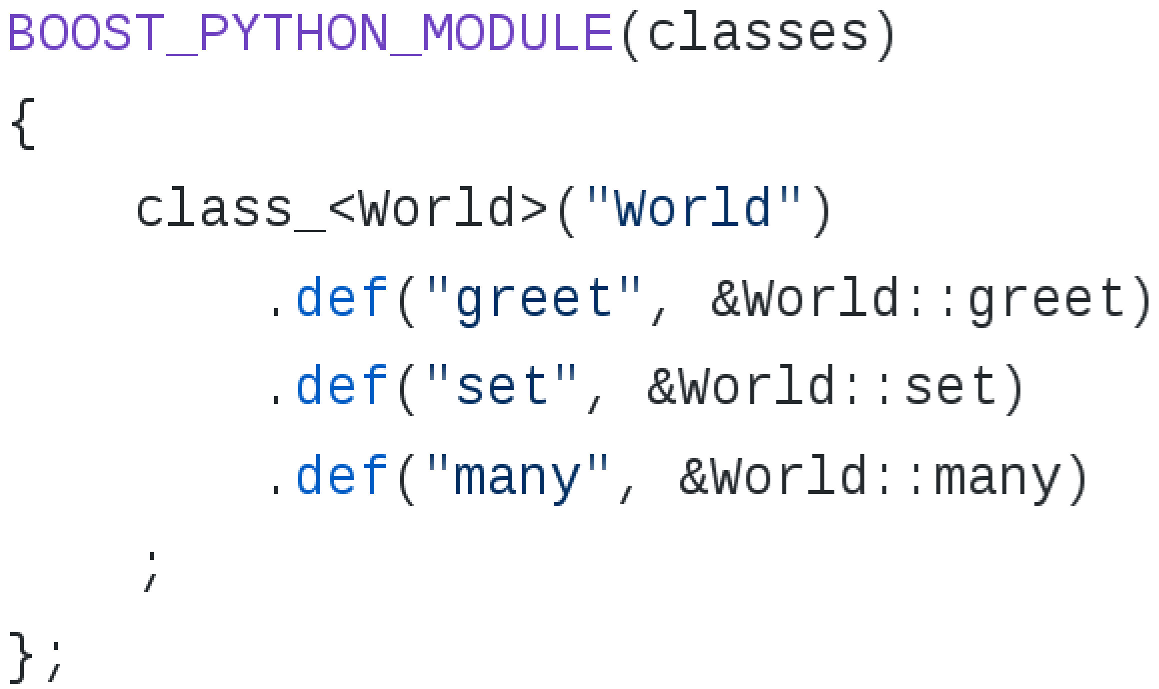
Compilation produces a dynamic library which python can import as a module:



```
>>> from myModule import *
>>> x=myRange(10)
>>> print x
[0, 1, 2, 3, 4, 5, 6, 7, 8, 9]
```

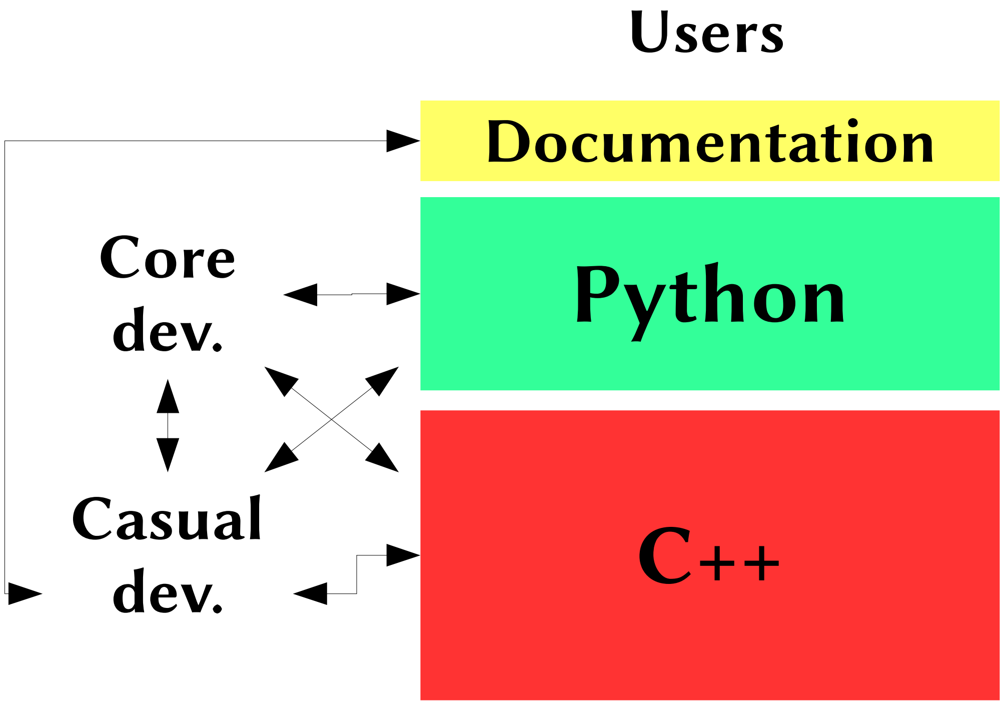
boost::python

Wrapping classes is also possible



```
BOOST_PYTHON_MODULE(classes)
{
    class_<World>("World")
        .def("greet", &World::greet)
        .def("set", &World::set)
        .def("many", &World::many)
    ;
};
```

A challenging development problem



Lots of interactions

+

Incompleteness of the interface

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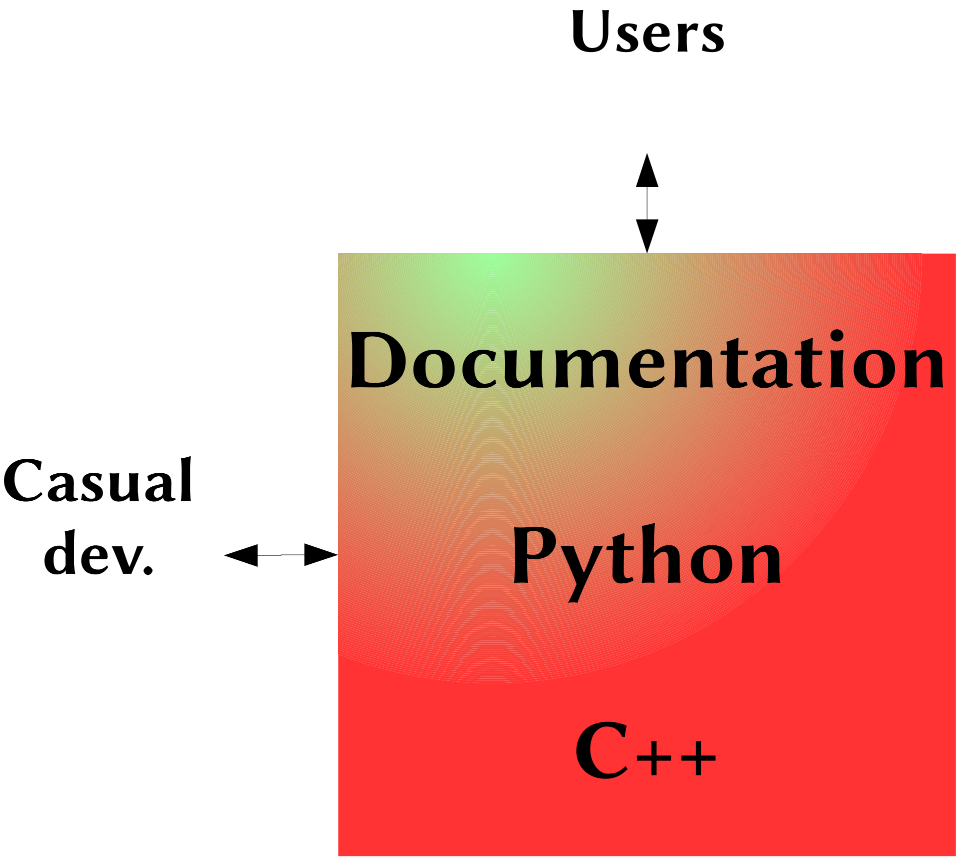
- **minimize workload**

A challenging development problem



Users

little to no time/experience in programming

Needs:

- documentation
- computational efficiency
- simplicity of usage
- flexibility
- interactivity

Casual devs.

want to implement something new (contact model, particle shape,...)

Needs:

- simplicity of implementation
- low commit barrier
- will hardly learn new programing techniques

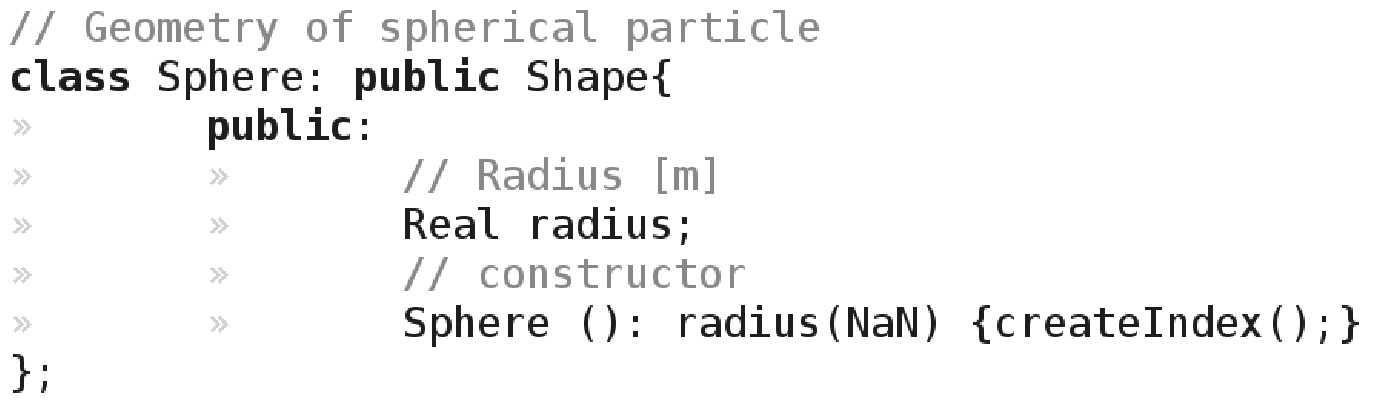
Core devs.

Needs:

- minimize workload

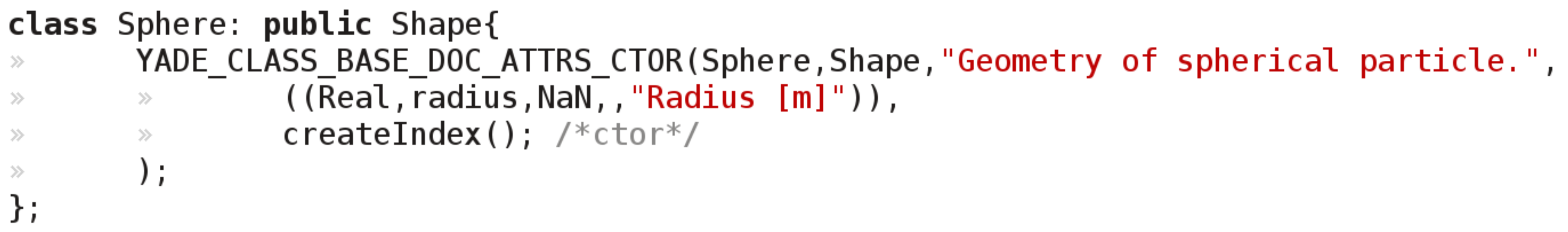
YADE_CLASS macro

Without python wrapping the class declaration of "Sphere" would be:



```
// Geometry of spherical particle
class Sphere: public Shape{
»       public:
»       »       // Radius [m]
»       »       Real radius;
»       »       // constructor
»       »       Sphere (): radius(NaN) {createIndex();}
};
```

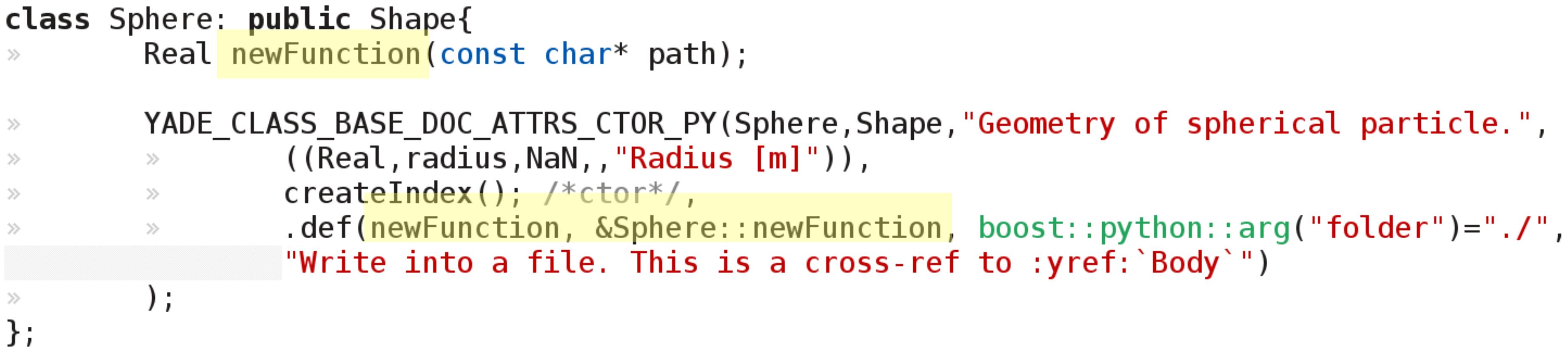
Yade is imposing a different form in which declaration, initialization, wrapping and documentation are simultaneous:



```
class Sphere: public Shape{
»       YADE_CLASS_BASE_DOC_ATTRS_CTOR(Sphere,Shape,"Geometry of spherical particle.",
»       »       ((Real,radius,NaN,,"Radius [m]")),
»       »       createIndex(); /*ctor*/
»       );
};
```

YADE_CLASS macro

Functions as well (and much more):



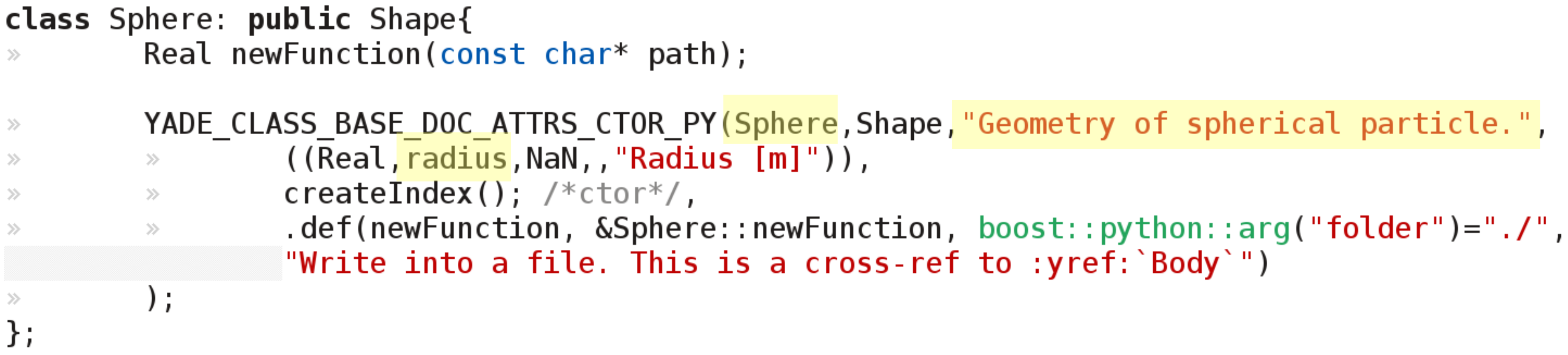
```
class Sphere: public Shape{
»       Real newFunction(const char* path);

»       YADE_CLASS_BASE_DOC_ATTRS_CTOR_PY(Sphere,Shape,"Geometry of spherical particle.",
»       »       ((Real,radius,NaN,,"Radius [m]")),
»       »       createIndex(); /*ctor*/,
»       »       .def(newFunction, &Sphere::newFunction, boost::python::arg("folder")="./",
                "Write into a file. This is a cross-ref to :yref:`Body`")
»       );
};
```

Result:

Python wrapping is a mandatory part of the class declaration, it appears in all header files

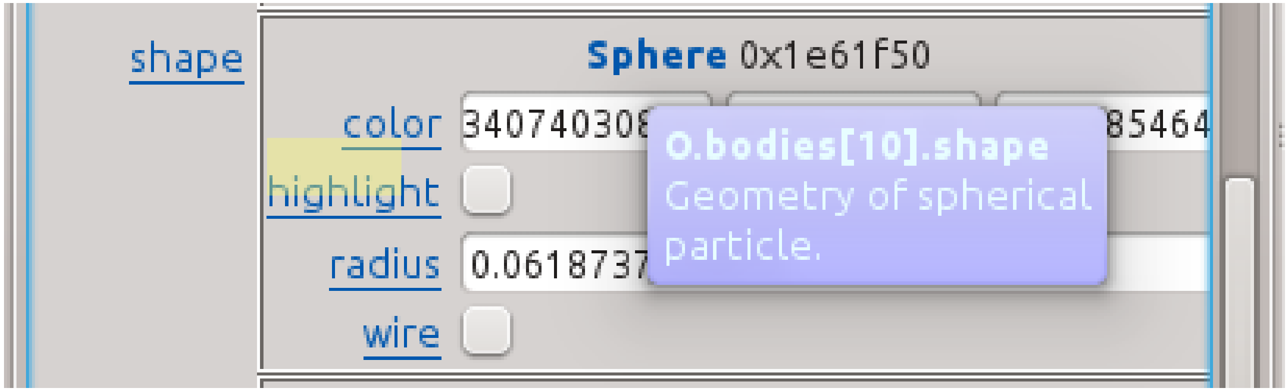
YADE_CLASS macro



```
class Sphere: public Shape{
»       Real newFunction(const char* path);

»       YADE_CLASS_BASE_DOC_ATTRS_CTOR_PY(Sphere,Shape,"Geometry of spherical particle.",
»       »       ((Real,radius,NaN,,"Radius [m]")),
»       »       createIndex(); /*ctor*/,
»       »       .def(newFunction, &Sphere::newFunction, boost::python::arg("folder")="./",
                "Write into a file. This is a cross-ref to :yref:`Body`")
»       );
};
```

In the Qt window:



shape

Sphere 0x1e61f50

color 340740308 … 85464

highlight □

radius 0.0618737

wire □

O.bodies[10].shape

Geometry of spherical particle.

YADE_CLASS macro

In the online/pdf documentations (built with Sphinx):

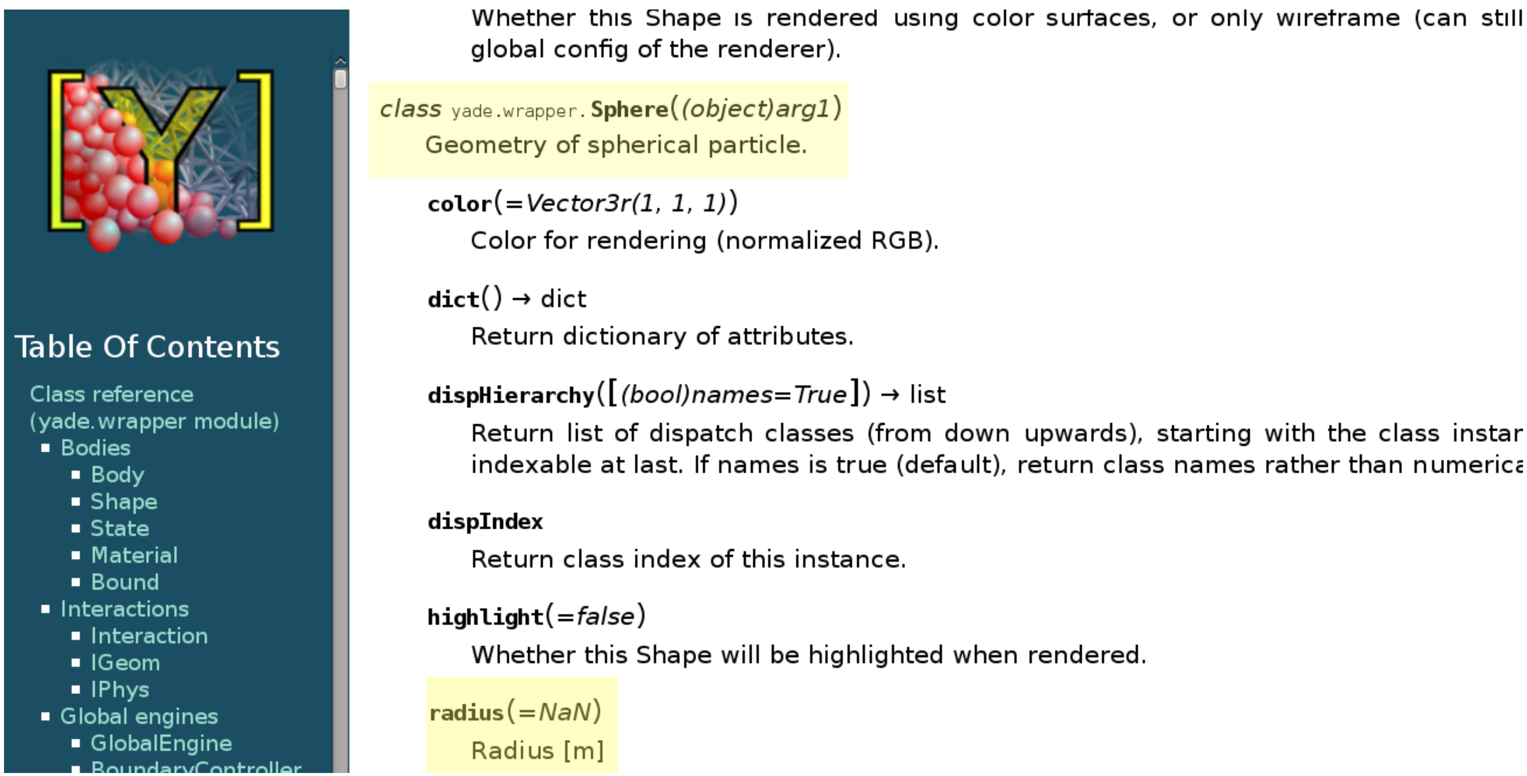


Table Of Contents

Whether this Shape is rendered using color surfaces, or only wireframe (can still global config of the renderer).

class yade.wrapper.**Sphere**(*(object)arg1*)
Geometry of spherical particle.

color(=*Vector3r(1, 1, 1)*)
Color for rendering (normalized RGB).

dict() → dict
Return dictionary of attributes.

dispHierarchy([*(bool)names=True*]) → list
Return list of dispatch classes (from down upwards), starting with the class instar indexable at last. If names is true (default), return class names rather than numerica

dispIndex
Return class index of this instance.

highlight(=*false*)
Whether this Shape will be highlighted when rendered.

radius(=*NaN*)
Radius [m]

YADE_CLASS macro

Inline documentation and auto-completion (ipython):

```
Yade [2]: s=Sphere()
Yade [3]: s?
Type:       Sphere
String Form:<Sphere instance at 0x354d800>
File:       /usr/lib/x86_64-linux-gnu/yadedaily/py/yade/wrapper.so
Docstring:  Geometry of spherical particle.

Yade [4]: s.
s.color          s.dispHierarchy  s.highlight      s.updateAttrs
s.dict           s.dispIndex      s.radius         s.wire

Yade [4]: s.radius?
Type:       property
String Form:<property object at 0x7f61aae16db8>
Docstring:  Radius [m] :ydefault:`NaN` :yattrtype:`Real` :yattrflags:`0`
```

Note: YADE itself is a python module

```
bchareyre@dt-med008:~$ yade
Welcome to Yade 1.07.0
TCP python prompt on localhost:9000, auth cookie `adkyus'
XMLRPC info provider on http://localhost:21000
[[ ^L clears screen, ^U kills line. F12 controller, F11 3d
view (use h-key for showing help), F10 both, F9 generator,
F8 plot. ]]
Yade [1]:
```

Behind the scene:

```
~$ python
In [1]: #set custom ipython decorations and other things
...
In [N]: import yade
Yade [1]:
```

Conclusion

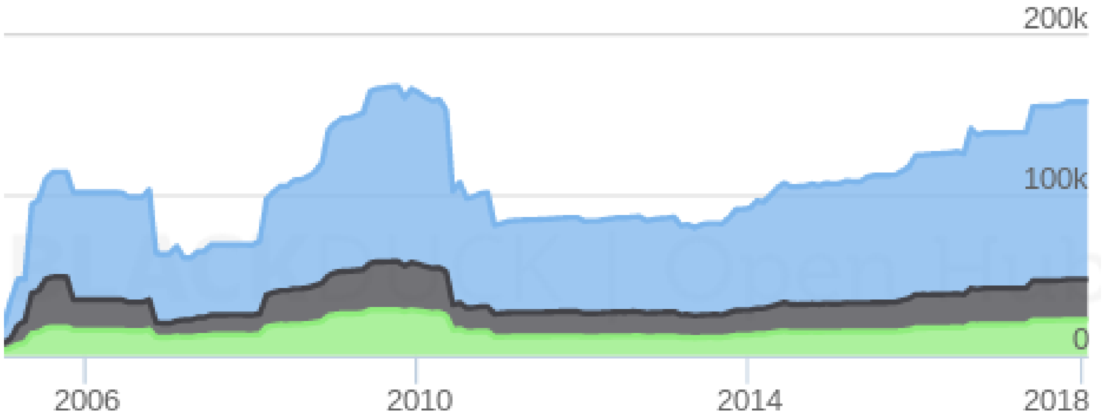
Advantages (among others)

- Nearly no limit to user's imagination
- Powerful (pre/post-)processing tools at no (development) cost
- Inline documentation
- Debugging scenes is much easier
- Couplings with other codes: OpenFoam, e-script (FEM), Yales2, Palabos,...
- Some task parallelism can be exploited at the python level (mpi4py for FEMxDEM)
- Online discussions and bug reports can come with Minimal Working Examples (MWE™)
- ...

Conclusion

Downside

- Very intrusive technique
- Compilation time skyrockets due to boost templates (~1h for fresh build on the average desktop)



Conclusions

- If you are starting an ambitious project in C++ better integrate python from the very beginning
- It may actually help for the development itself
- Yade-DEM could be used as a template project for such thing

Dependencies (some of them)

IP[y]:
IPython

CLI

NumPy

Math

matplotlib

Plotting

Eigen

Linear algebra

CGAL

Comput. Geometry

boost
C++ LIBRARIES

Everything

OpenBLAS
An optimized BLAS library

Optimized algebra

SuiteSparse

Sparse linear solvers

git

VCS

SPHINX
Python Documentation Generator

Python doc

Qt

GUI

OpenGL.

3D rendering

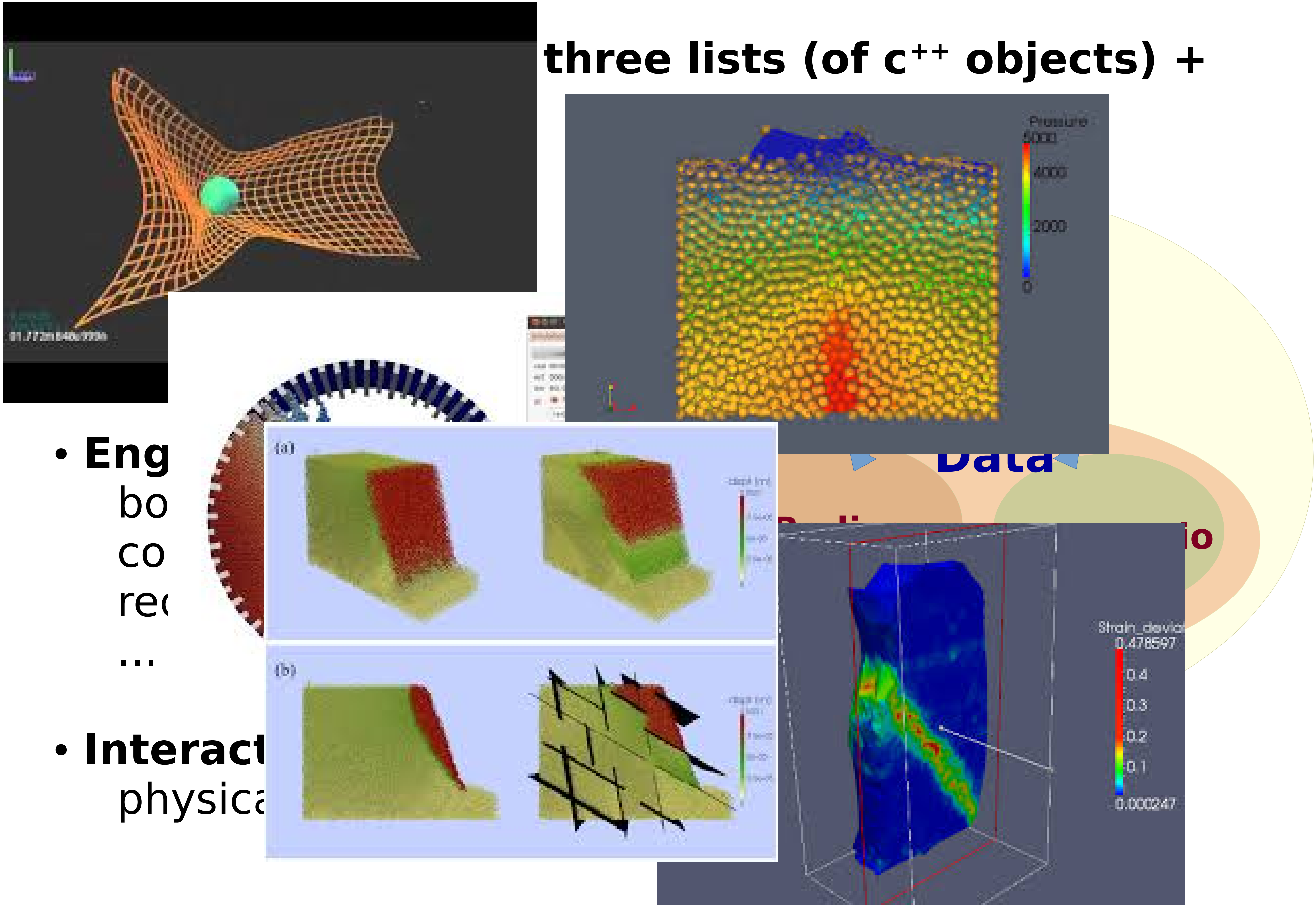
QGLViewer

VTK ParaView
Kitware

Post-processing

Scene & interface(s)

three lists (of c^{++} objects) +



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- **Interact**
  physica