The Swy Project

2. What is it?

1. What do we want it to be?

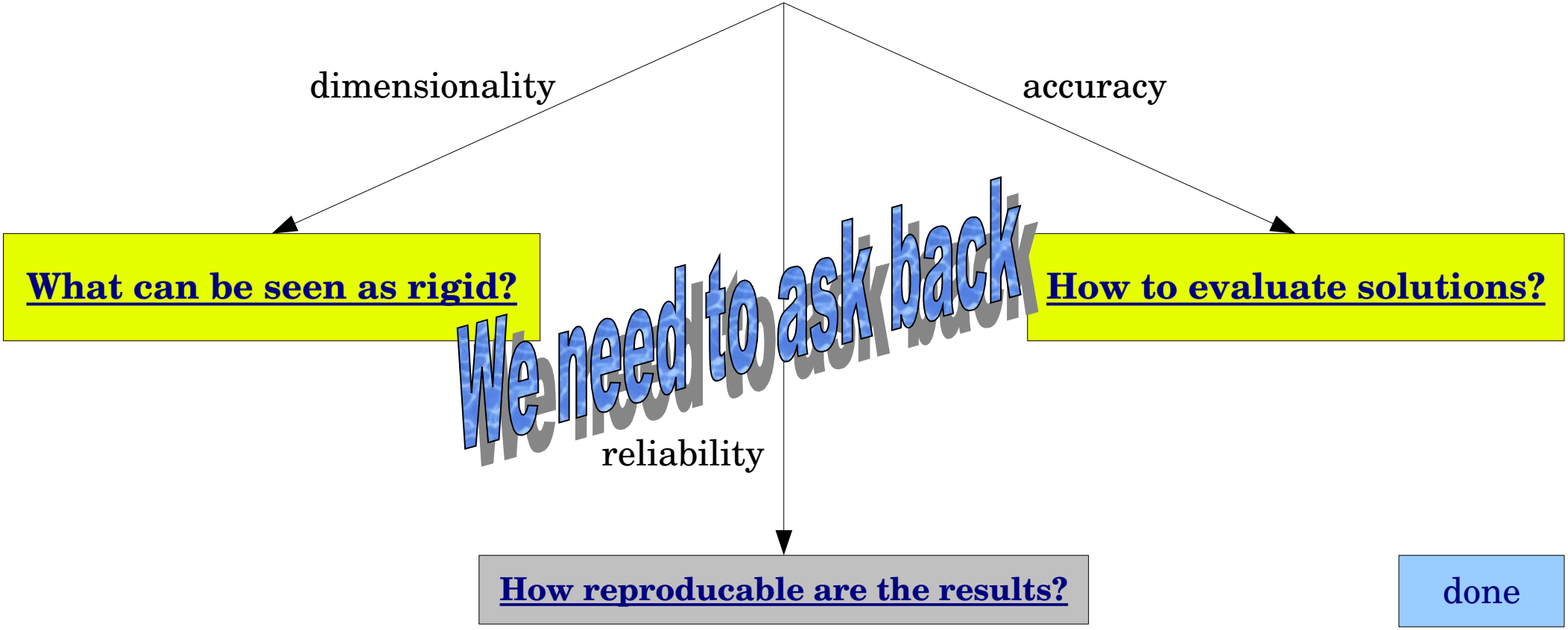
Let's explore it

Problem: Global Structural Optimization

→ **Question:** What does the user want to know? → everything

→ **Question:** What does the user NEED to know?

→ **Restrictions**



What can be seen as rigid?

Defines our search space

Possible answers:

- **Whole molecules → supramolecular**
- **Bond lengths / angles → dihedral**
- **Nothing → complete manipulation**

(could e.g. be tackeled with MD)

back

What can be seen as rigid?

Defines our (energy)calculator

Possible answers (in principal):

- **Single point calculations**
- **Optimizations**
- **MD simulations (and take snapshots or sth)**

In this case relevant: package, method, basis...

We expect a user to know what to choose

back

How reproducable are the results?

Defines just the numberOfRuns

back

Do we need more information to run a job?

We should not!

Easy to use

We have:

- **Search space**
- **(energy)Calculator**
- **numberOfRuns**

What about the metaHeuristic???

The metaHeuristic

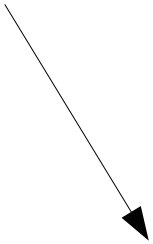
Corresponding question:

How to generate solutions?

What can be seen as rigid?
How to evaluate solutions?
How reproducable are the results?

Possible answers:

- **The Program should know!**



The Program should choose heuristic and parameters

by itself

And what does it look like atm?

What does the code look like?

Let's just look at the code directly
and follow what the computer does...

...starting with the input...

...and always comparing to what we want

Back to the start