# How to Professionally Develop Reusable Scientific Software—And When Not To

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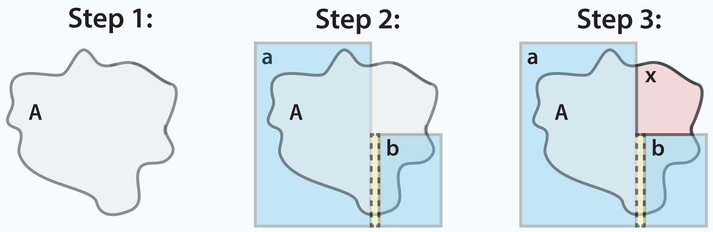
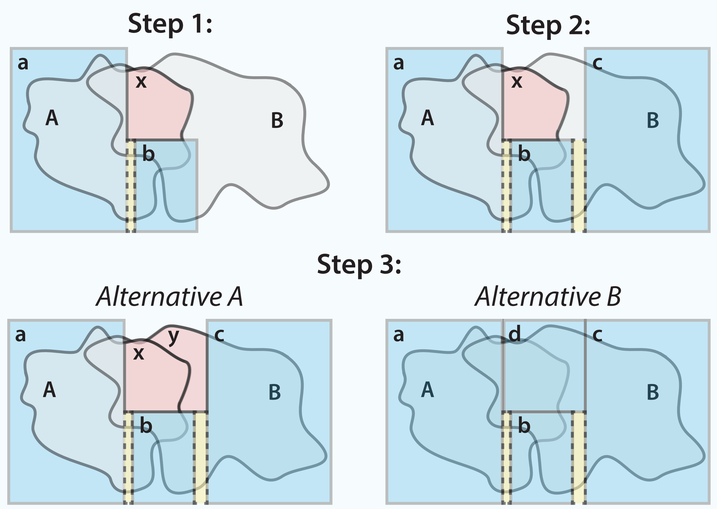
## Developing Computational Solutions

In theory, computational projects would be perfectly scoped from the start, allowing exact determination of what existing tools could be used and the reuse potential of new developments. In practice, project scopes change constantly, making it extremely difficult to accurately assess which code will be reused.

### Timeline: Problem A




### Timeline: Problem B




Solving a computational problem (grey) involves:

- finding existing well-defined packages (blue)
- implementing missing pieces with one-off prototype code (red)
- writing adapters (yellow) to interface between packages and protoypes

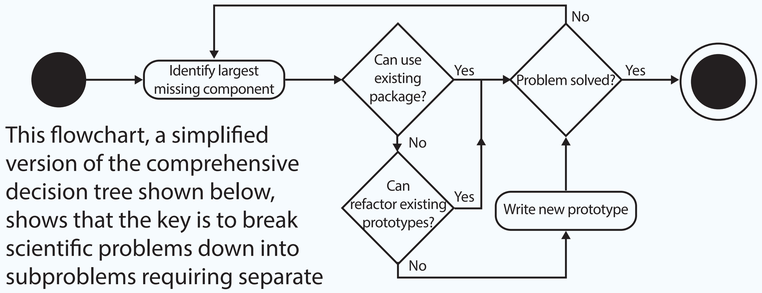
There are two options when existing prototypes solve part of the problem:

- implementing new protoypes to fill the holes (Alternative A)
- refactoring existing prototype into a package (Alternative B)

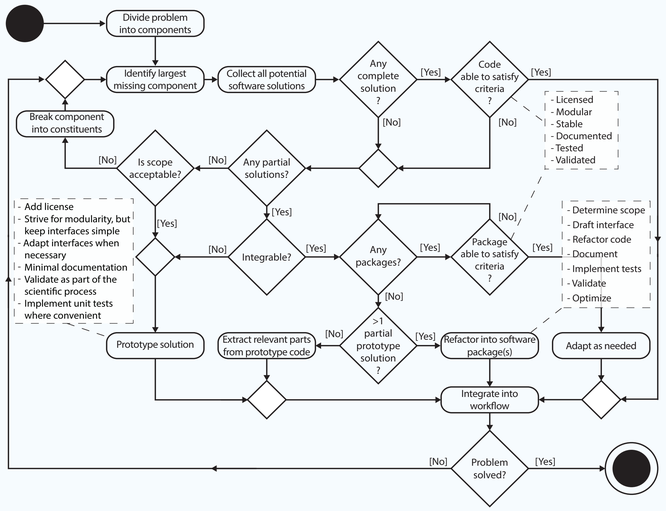
Determining when to choose each alternative and how to proceed is the crux of our lazy refactoring approach.

## Applying Lazy Refactoring

The lazy refactoring approach involves constantly reevaluating existing software whenever a new computational problem arises.




This flowchart, a simplified version of the comprehensive decision tree shown below, shows that the key is to break scientific problems down into subproblems requiring separate software solutions. These are analyzed to determine whether existing code, preferably in package form, can be used to solve them. New code, when needed, is always a prototype.



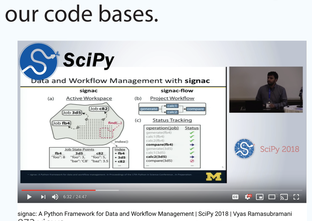

## Community Development

By presenting our open-source software in various forums, we

- attract a broad base of users and contributors
- help integrate our software with the broader ecosystem
- improve our software stack's usability and sustainability

We also foster group involvement in development by, for instance, holding periodic hackathons to upgrade and maintain our code bases.



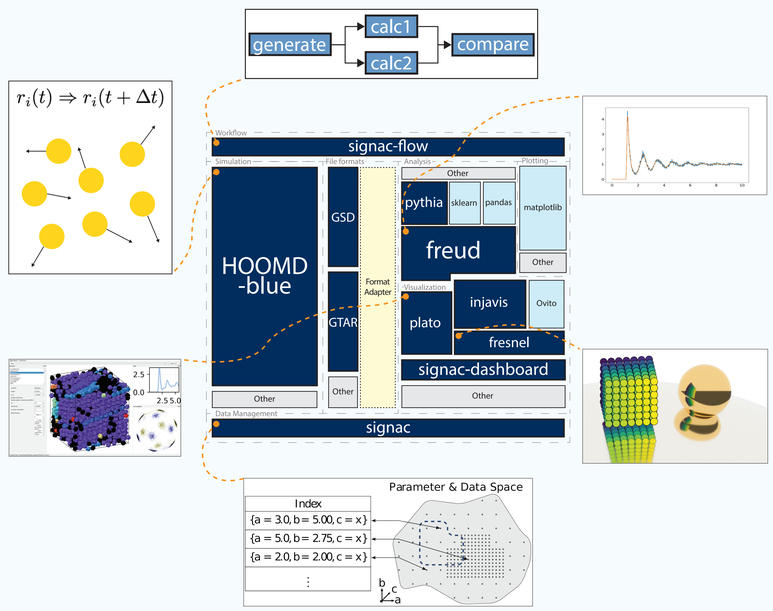



## Lazy Refactoring Over Time

Lazy refactoring has led to clear interfaces between well-defined groups of software tools that we developed in-house (navy blue):

- Molecular simulation: HOOMD-blue
- Simulation analysis: freud, pythia
- Simulation visualization: plato, injavis, fresnel
- Data and workflow management: signac, signac-flow, signac-dashboard
- Utilities: GSD, GTAR

These tools also interoperate with well-known components of the broader scientific Python ecosystem (light blue).




In addition to creating and maintaining these code bases, we also provide various other services to facilitate the broader usage of our code, such as:

- project websites including information on how to cite our code
- online documentation hosted through services like Read The Docs
- distribution through package managers like pip and conda
- support chat rooms (like Gitter) and mailing lists (like Google Groups)

Providing such services increases our visibility, and consequently the likelihood that others can reuse our work to accelerate scientific progress.

## Acknowledgements

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