Enabling open-source analytics in the enterprise

Michael Lawrence (Genentech Research)

August 16, 2018

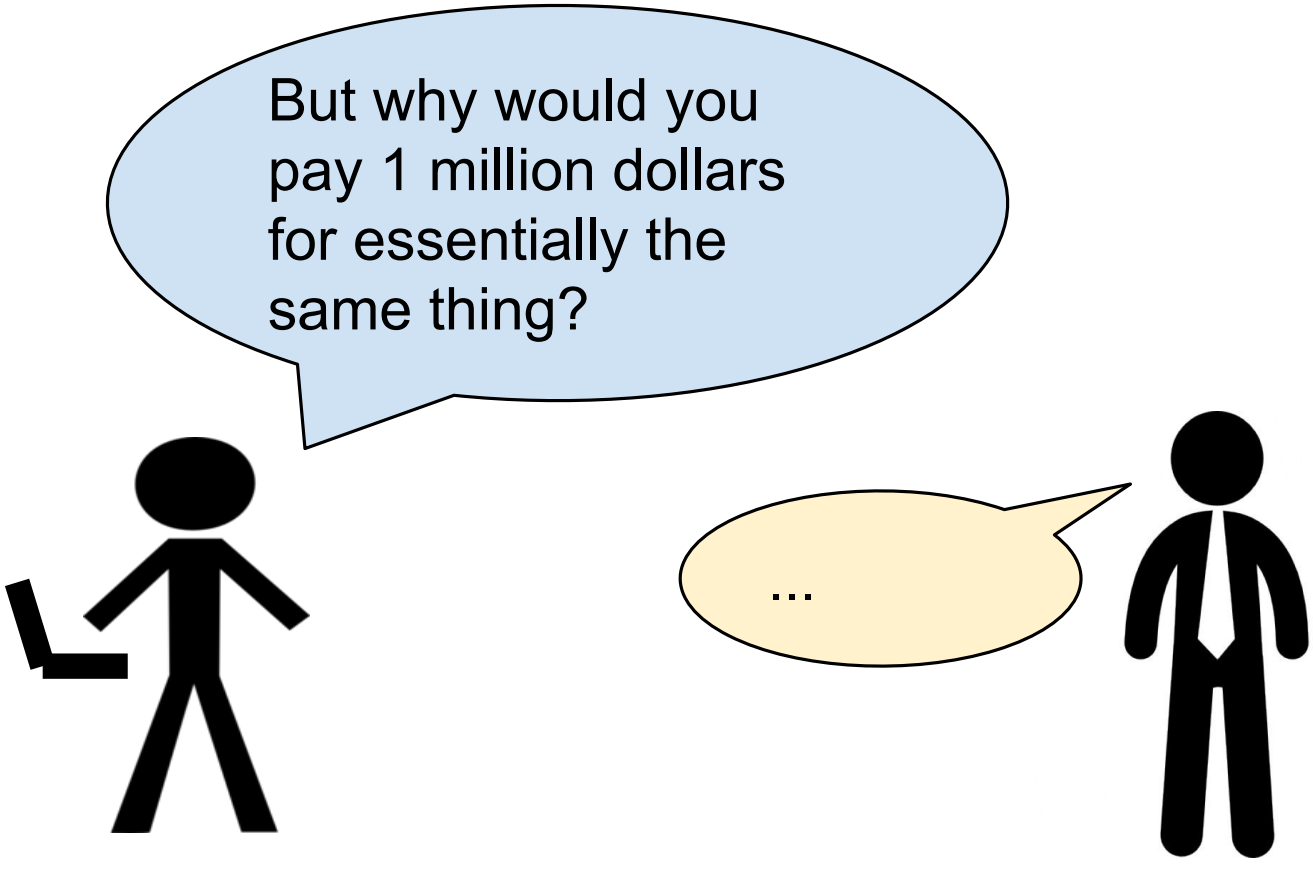
R is awesome

- R is free
- R is extensible and programmable
- R has thousands of high quality packages
  - Enable R to support virtually all research in statistical methods with minimal work by the core group
  - Enable reproducibility through versioning, ease of installation

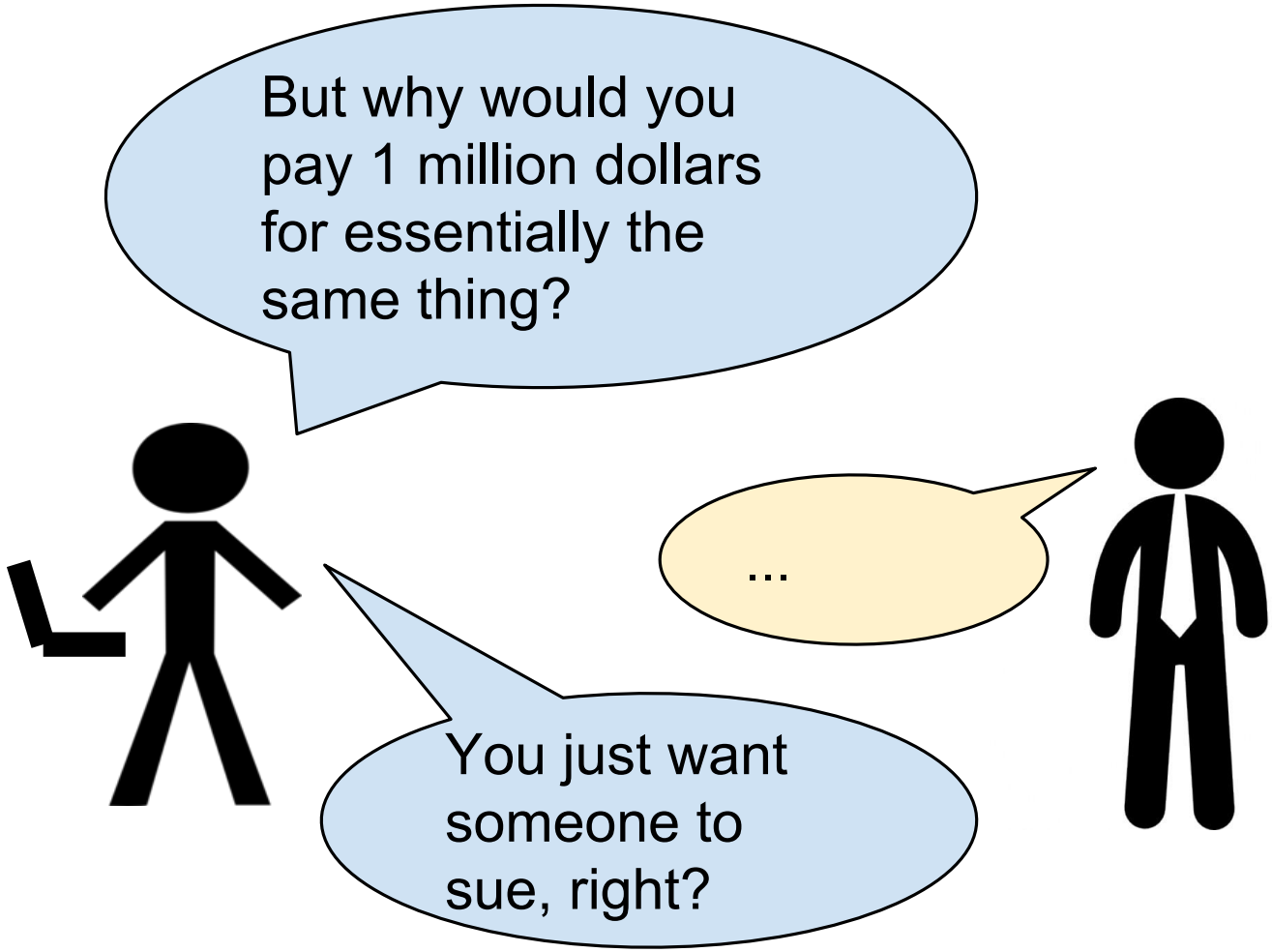
R is free!


I downloaded R onto my laptop and it was so easy to make this plot..
Yea.. but we're going with company X

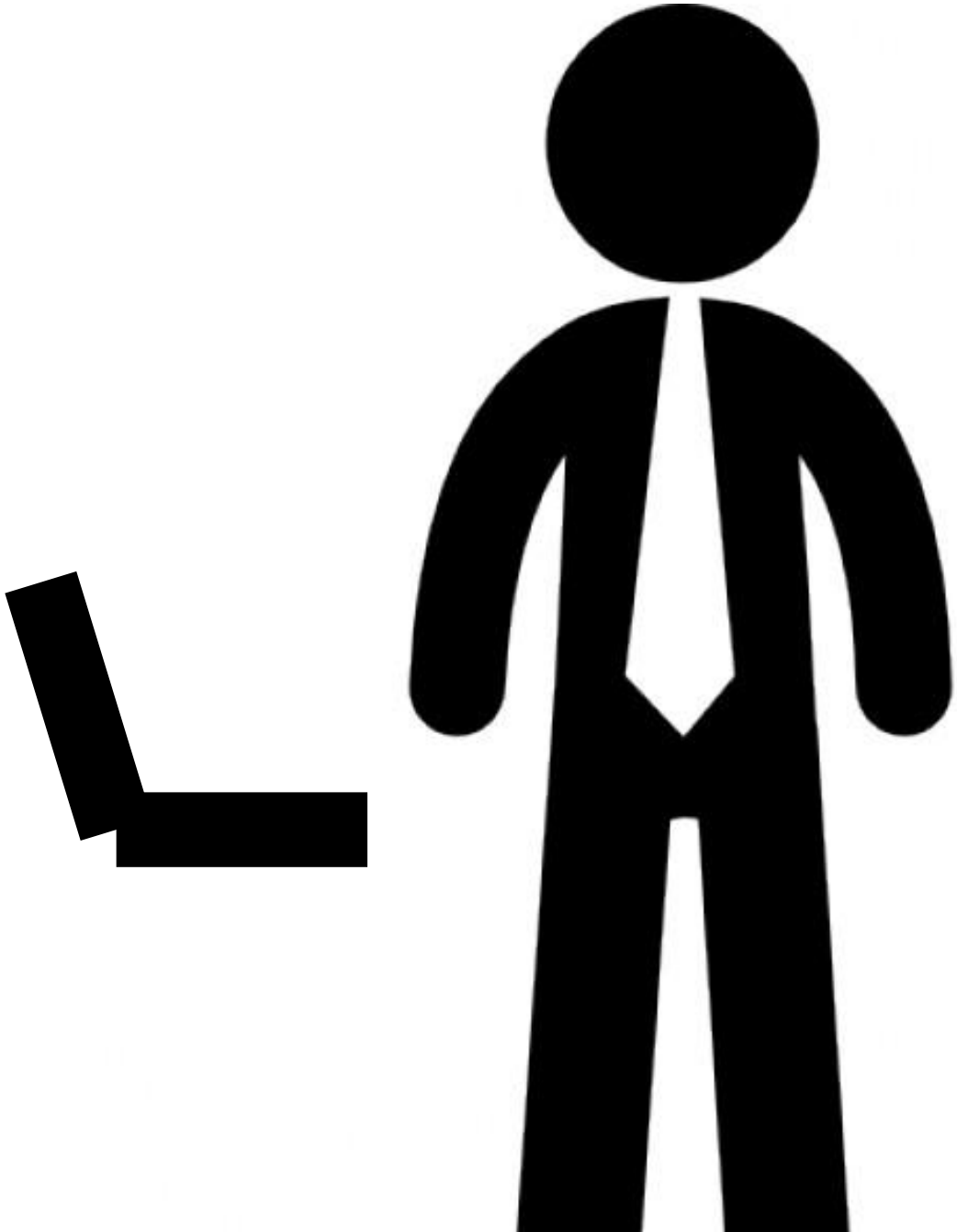
R is free!


But why would you pay 1 million dollars for essentially the same thing?
...

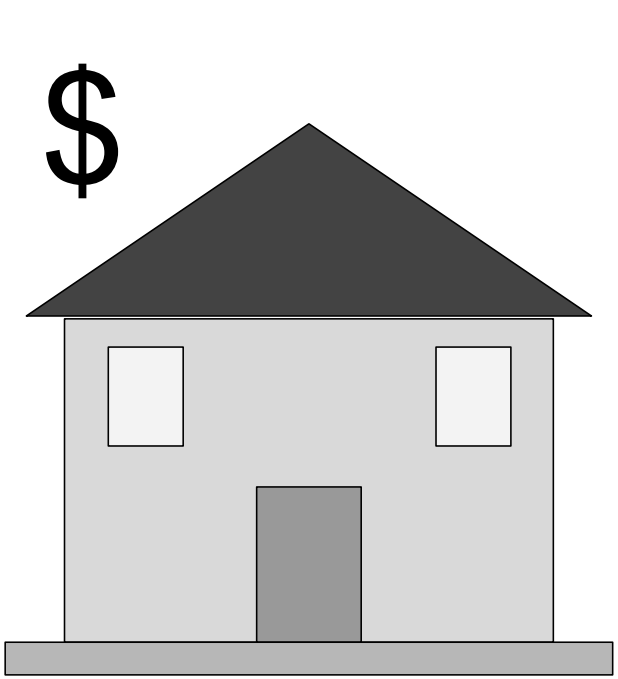
R is free!


But why would you pay 1 million dollars for essentially the same thing?
...
You just want someone to sue, right?

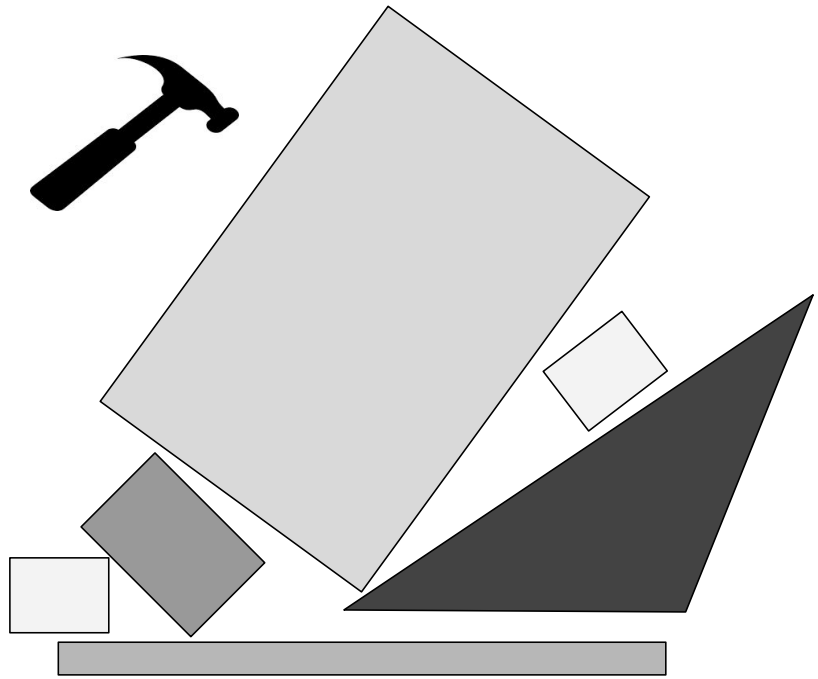
Playing devil's advocate



Build vs. buy

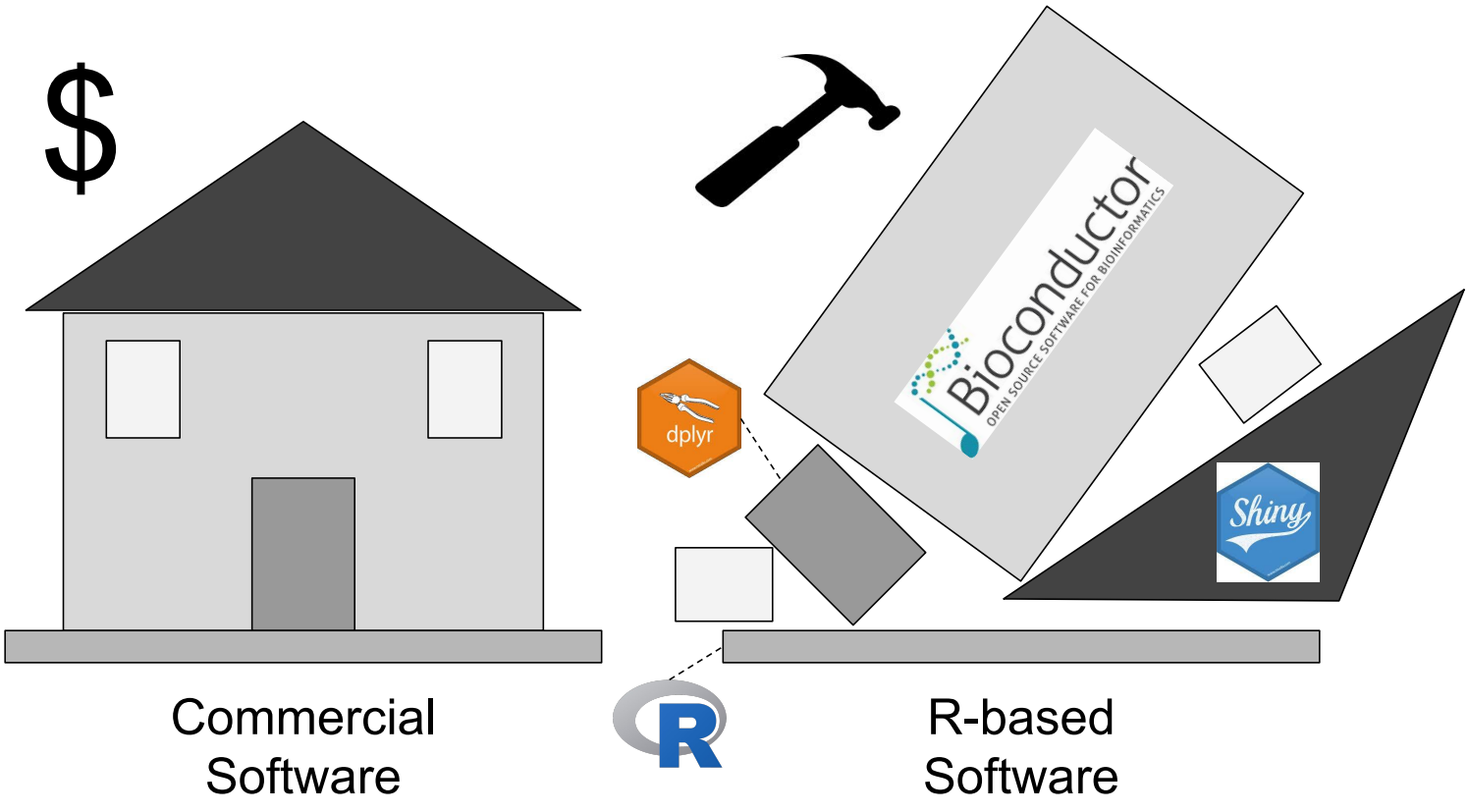


Commercial Software

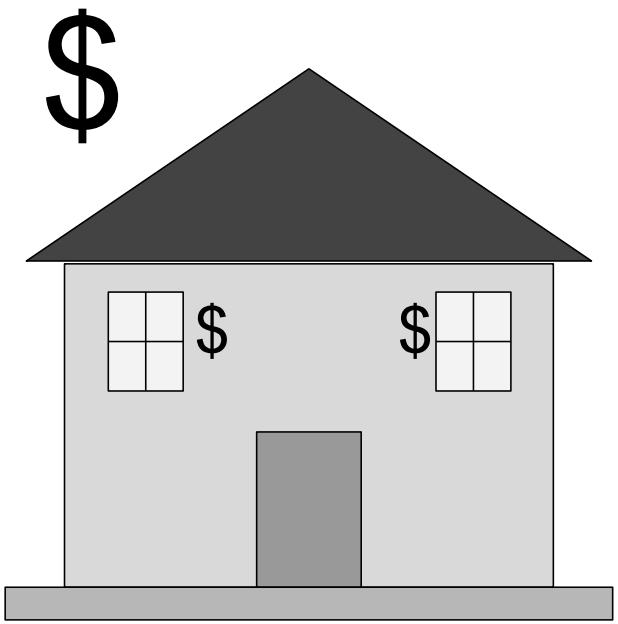


R-based Software

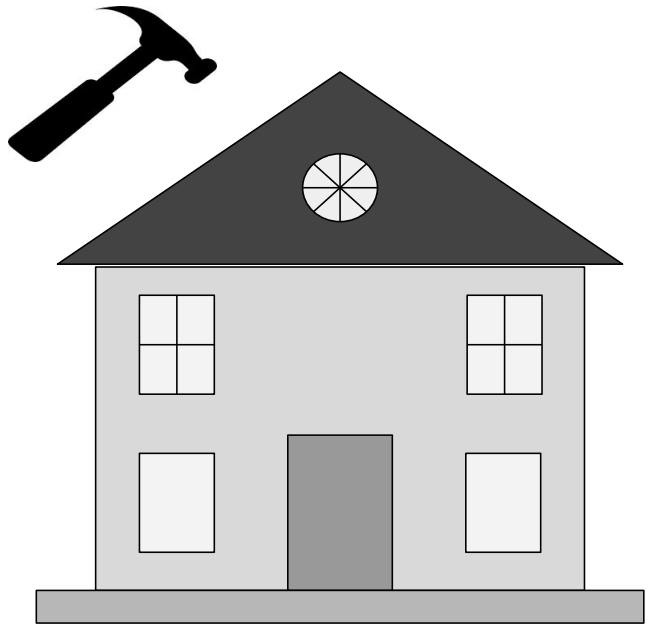
Build vs. buy


$
dplyr
Bioconductor
OPEN SOURCE SOFTWARE FOR BIOINFORMATICS
Shiny
R
Commercial Software
R-based Software

Build vs. buy

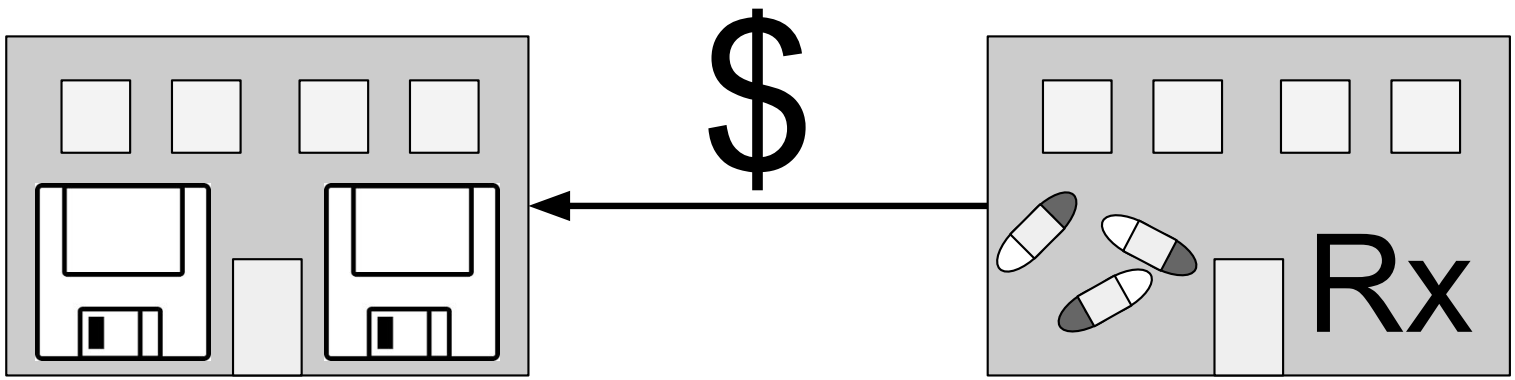


Customized
Commercial Software



Customized
R-based Software

From *paying* a software company...

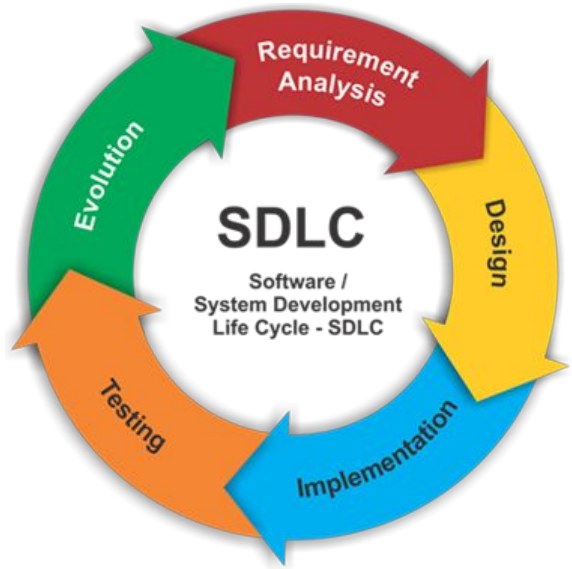


. . . to *being* a software company

R's strengths are also its weaknesses

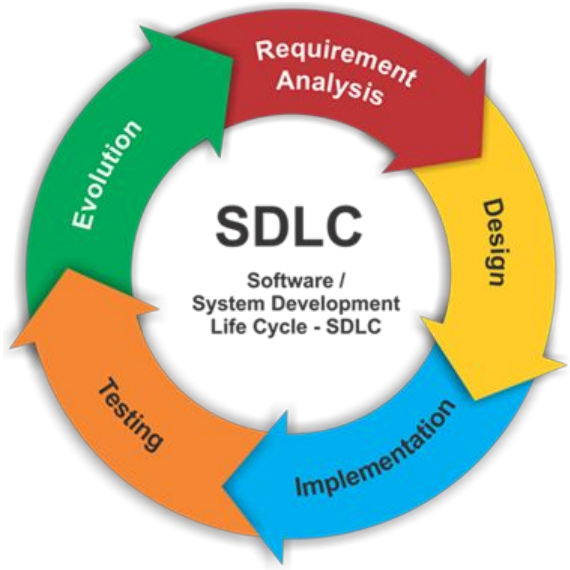
- ~~R is free~~ R is an investment
- ~~R is extensible and programmable~~ R needs to be programmed
  - How do we develop software for science?
    - That enables collaboration across the scientific enterprise?
- ~~R has thousands of high quality packages~~ R has too many packages
  - How do we manage our R environment?

Gated evolution: The scientific software lifecycle



Gated evolution: The scientific software lifecycle

Inception
(during scientific inquiry)

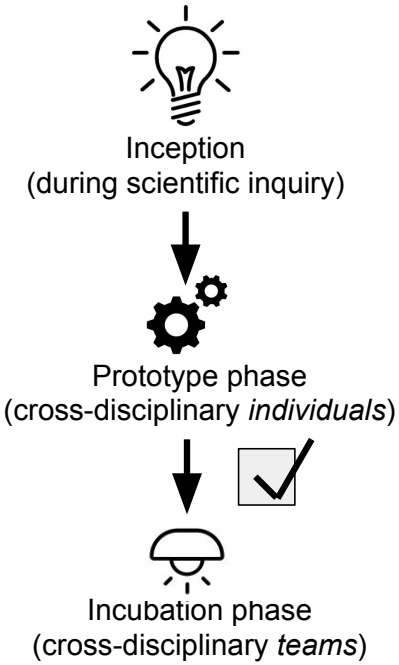


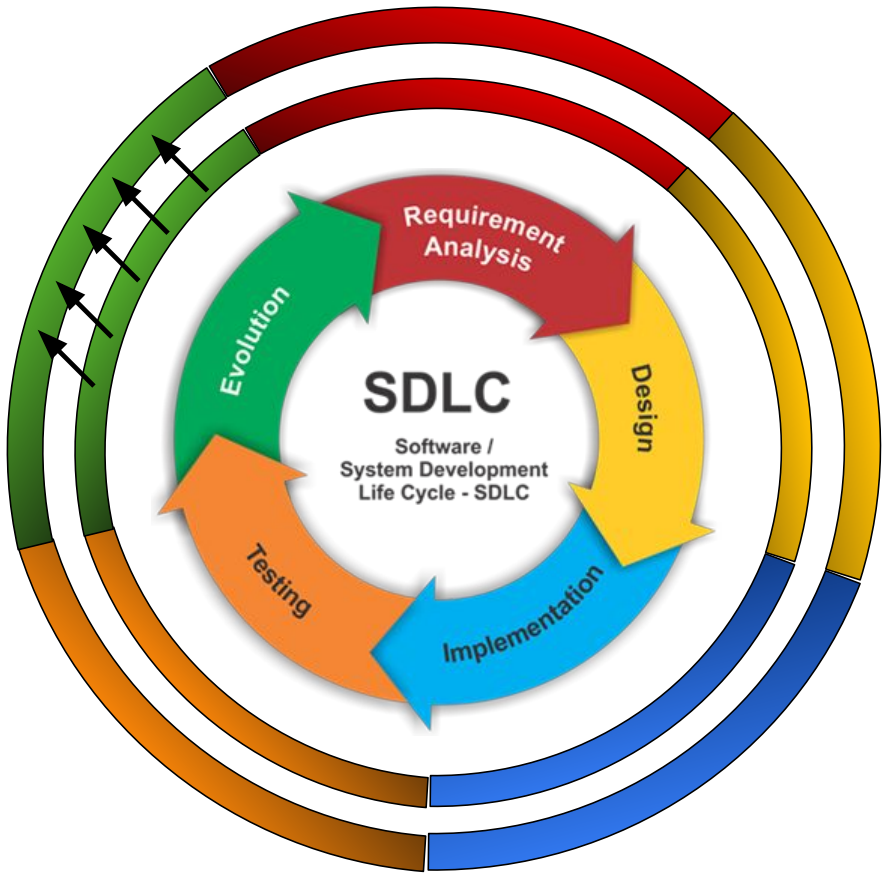
Gated evolution: The scientific software lifecycle

Inception
(during scientific inquiry)

Prototype phase
(cross-disciplinary *individuals*)

Gated evolution: The scientific software lifecycle





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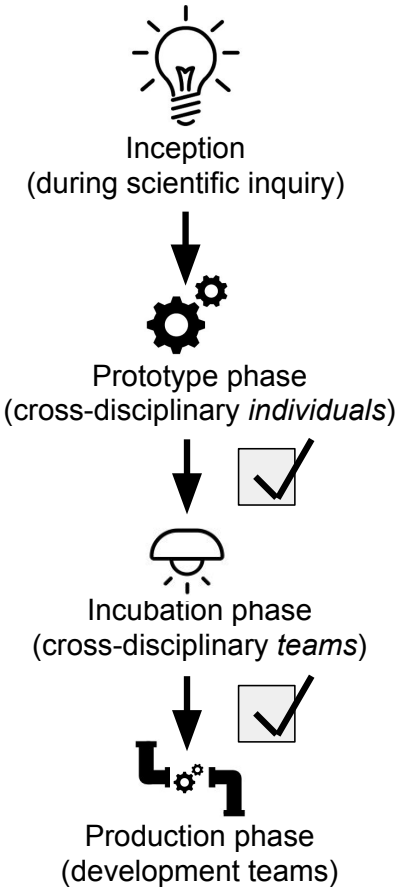

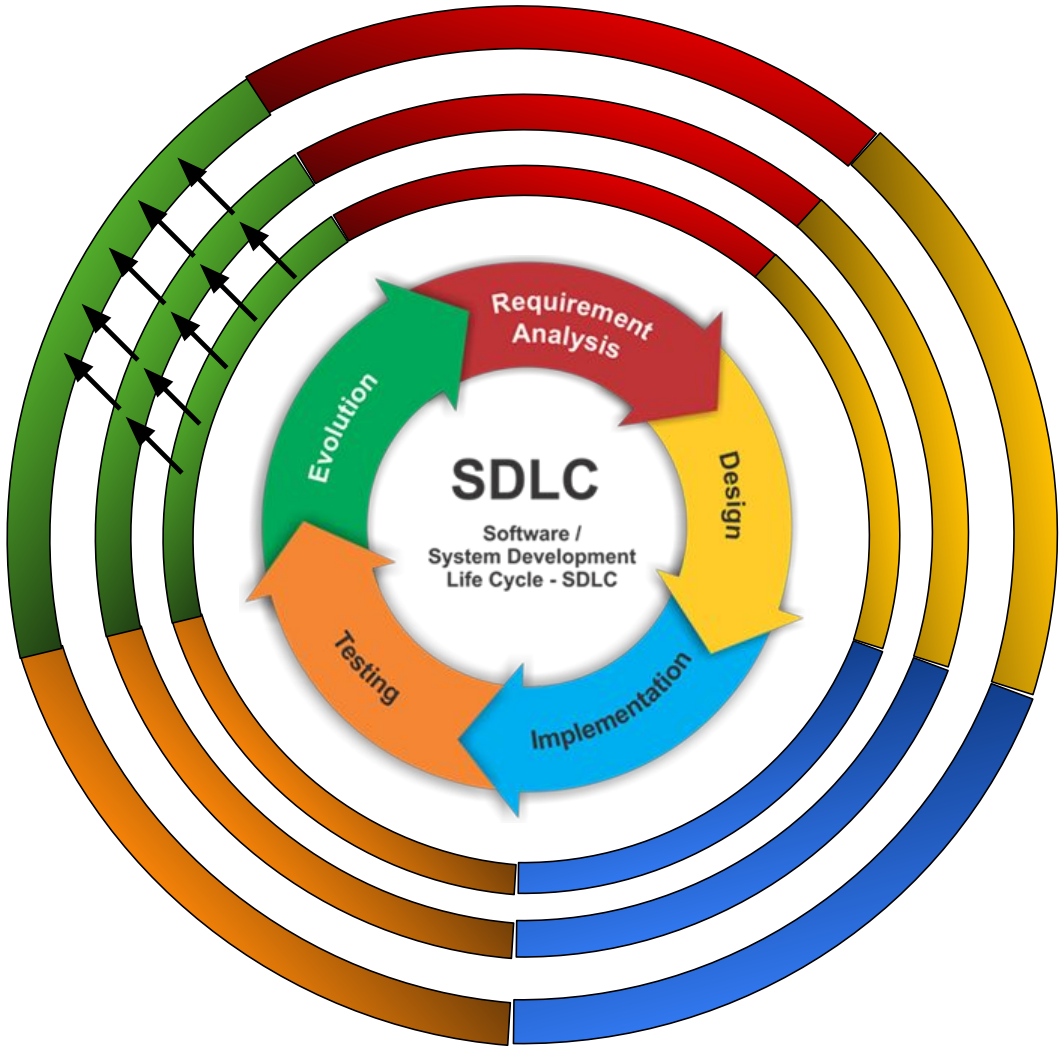

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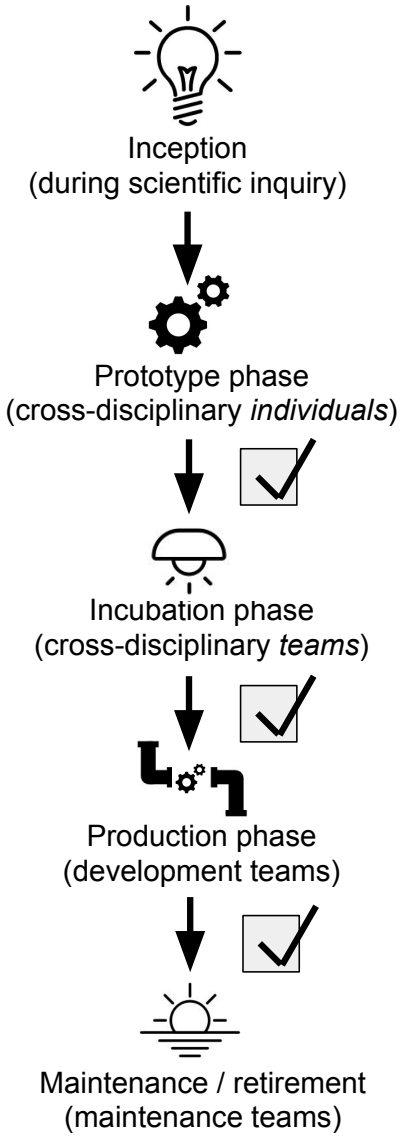

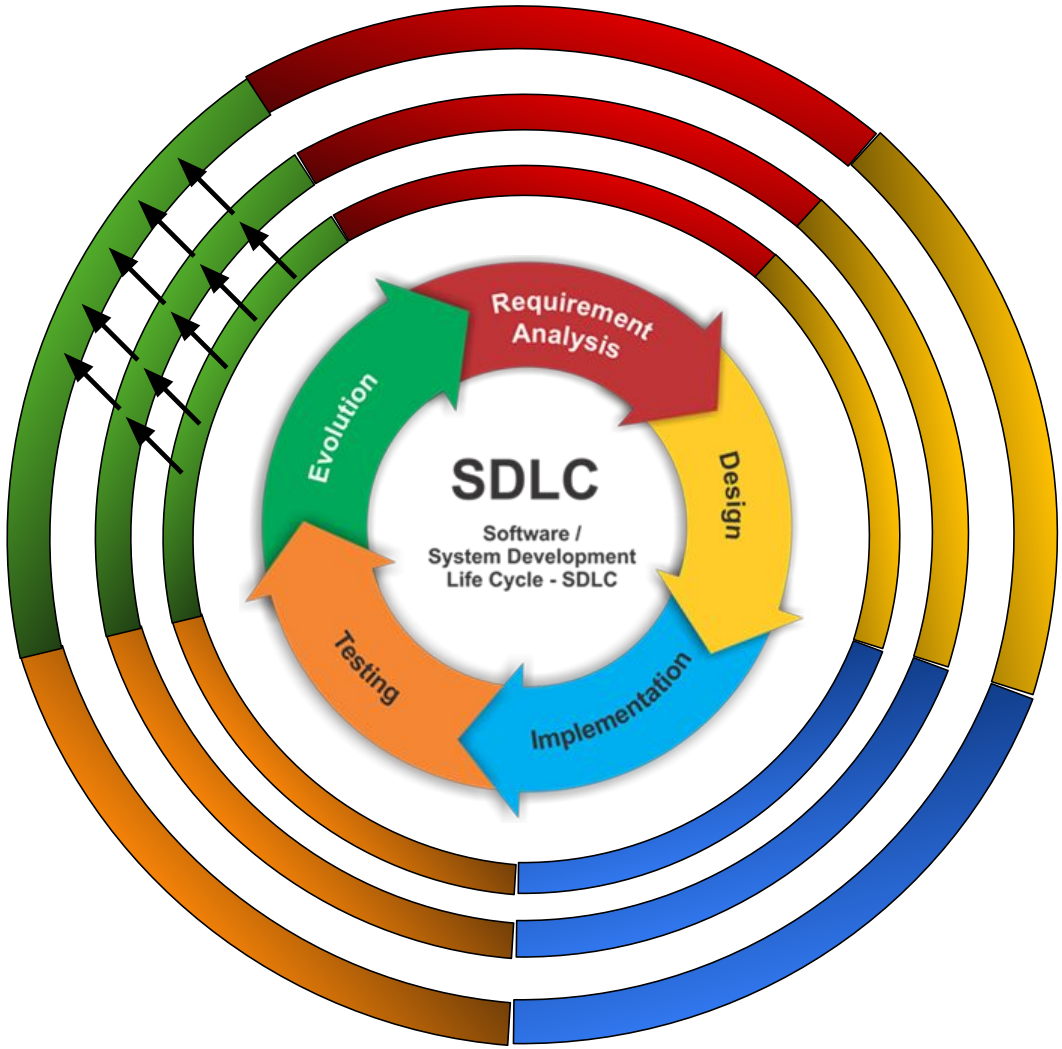

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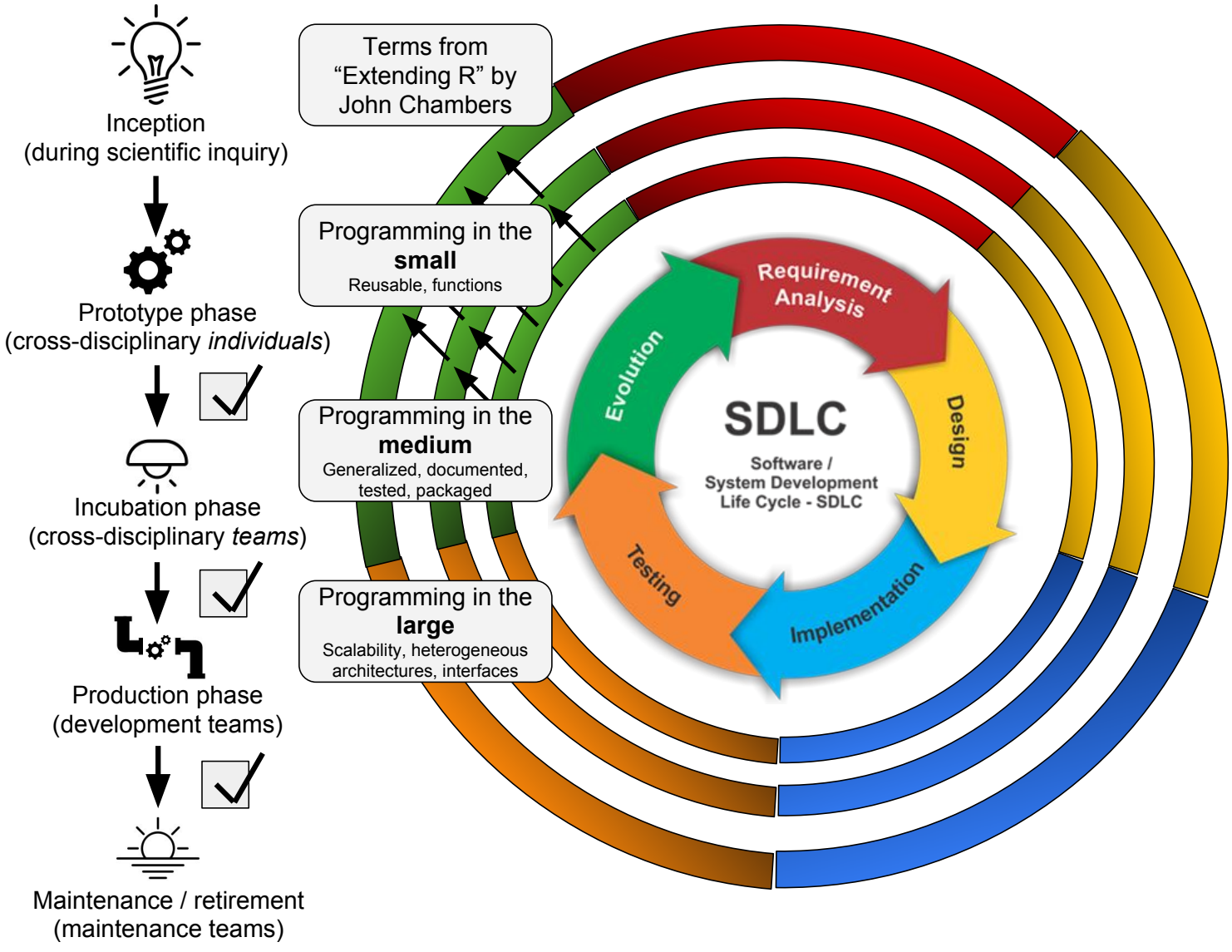
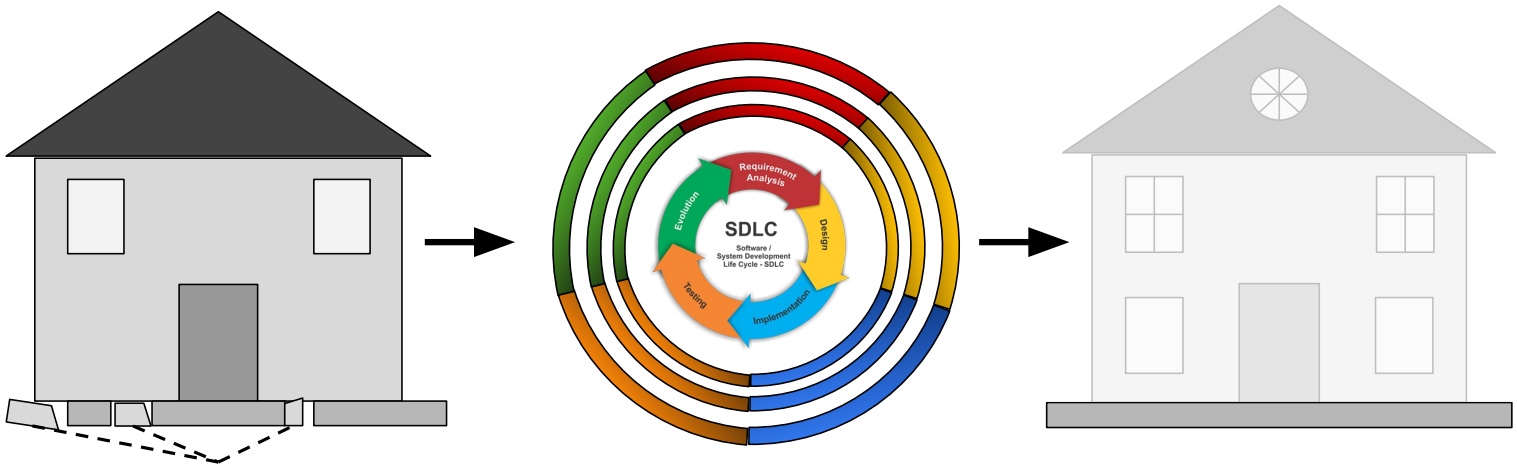


The incubator feedback loop

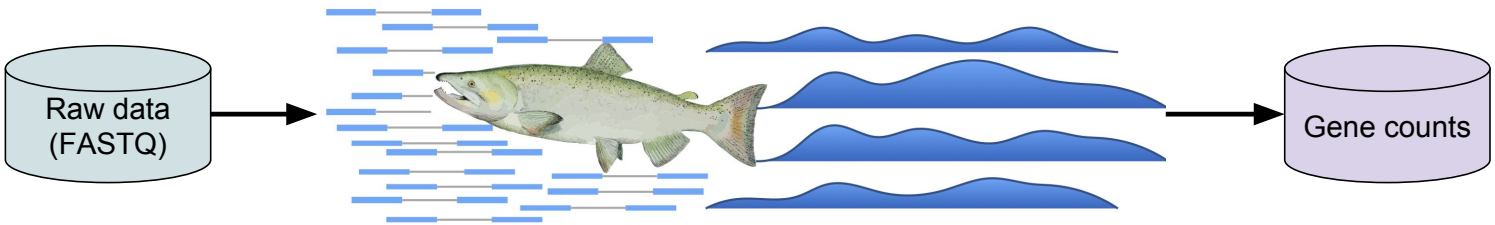


Infrastructure gaps

Incubation Process

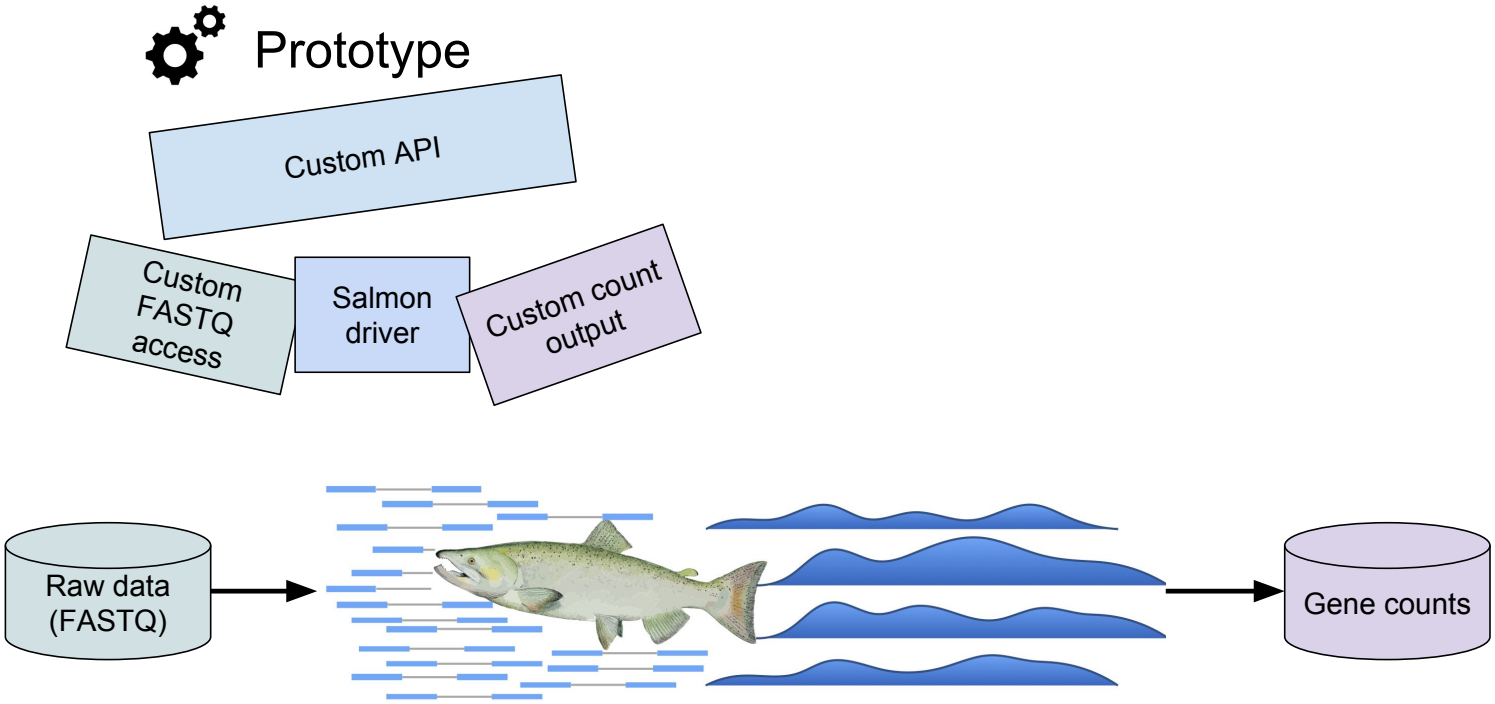
Gaps filled for future prototypes

Incubation example: gSalmon



Salmon (Public tool for RNA-seq expression counting)

Incubation example: gSalmon



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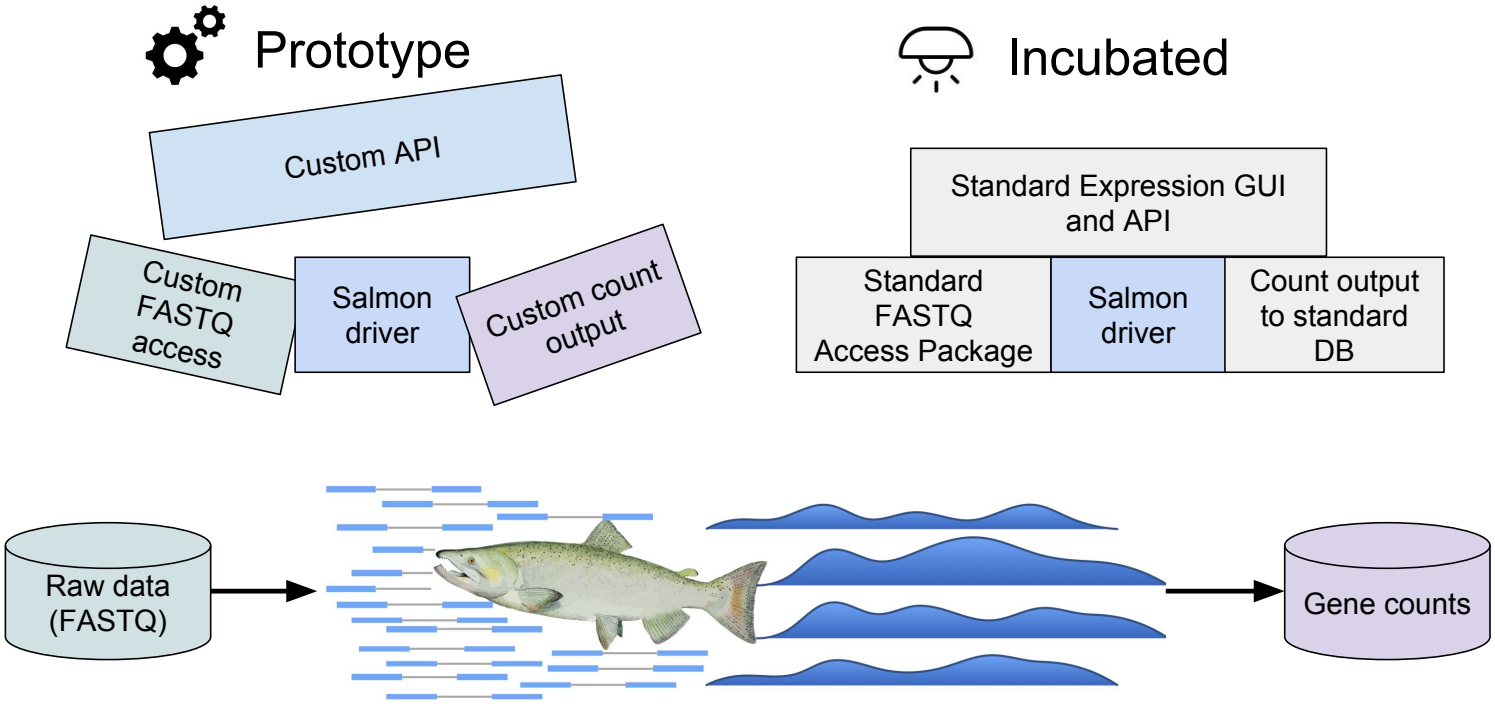

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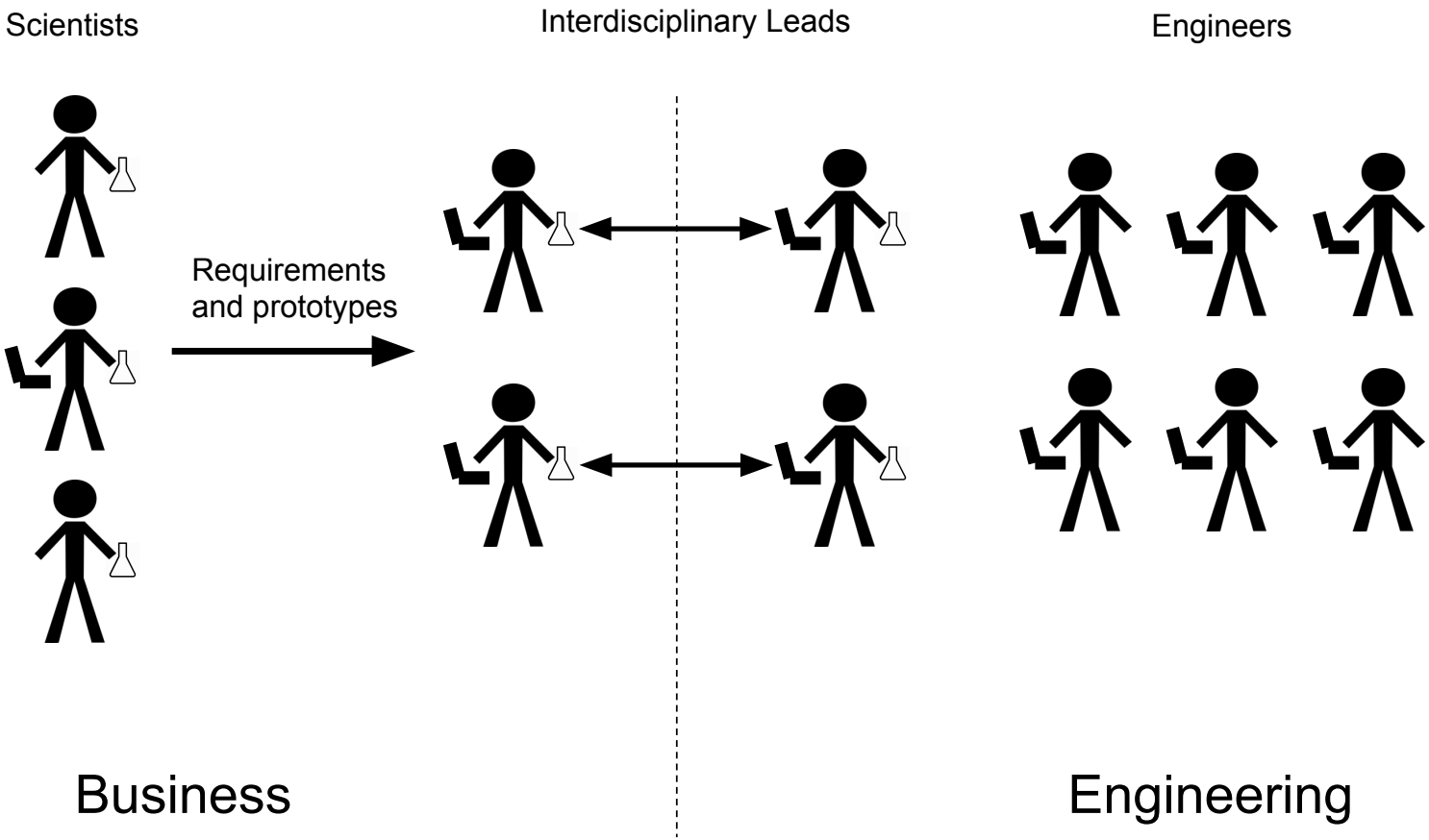
Managing developer resources



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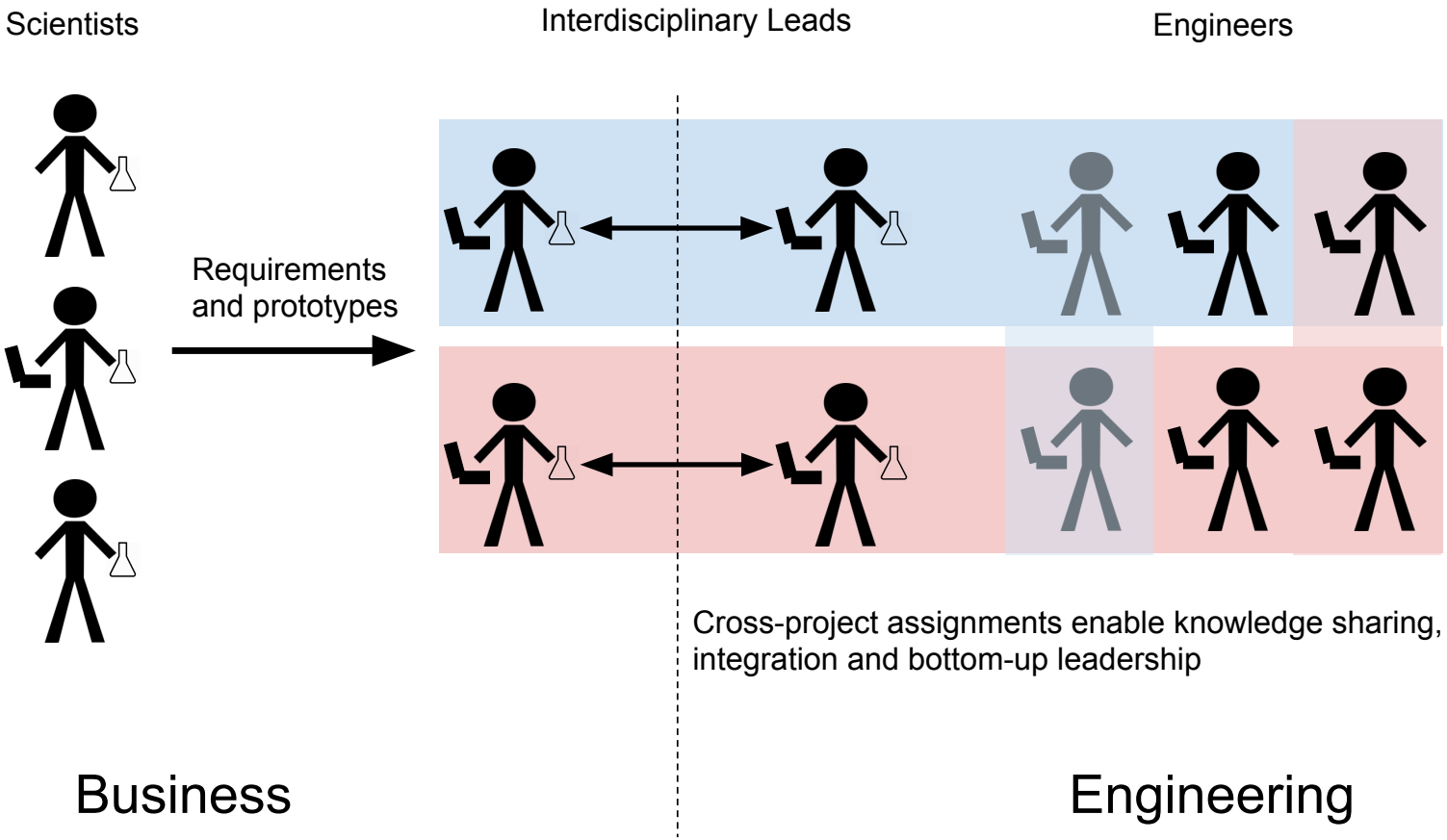

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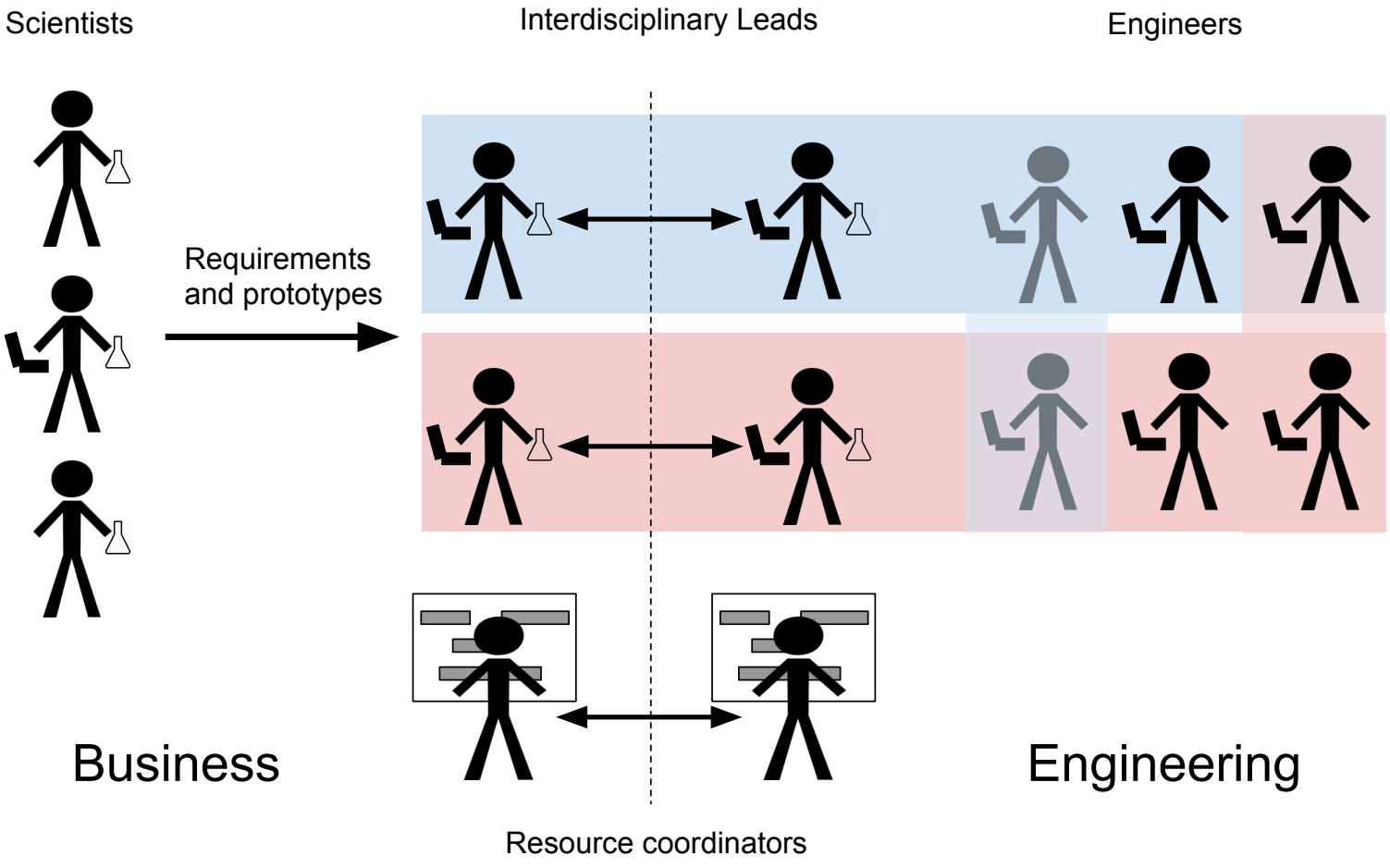


Contributing back to open-source

the engineering case

- Setting out to open-source puts the right perspective on development and leads to better software
- Lets us steer open-source development:
  - Specific projects
  - Trend setting, across the field

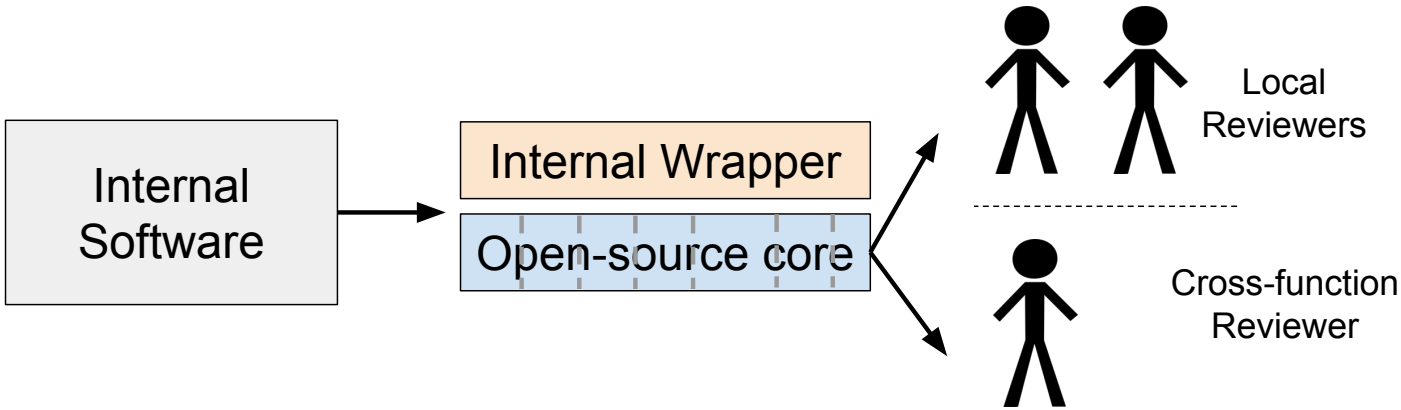
Contributing back to open-source

the scientific case

- Open-source software publication is an intellectual contribution to science, equivalent to a paper
- Enhances potential for collaborations
- Enables reproducibility of published results

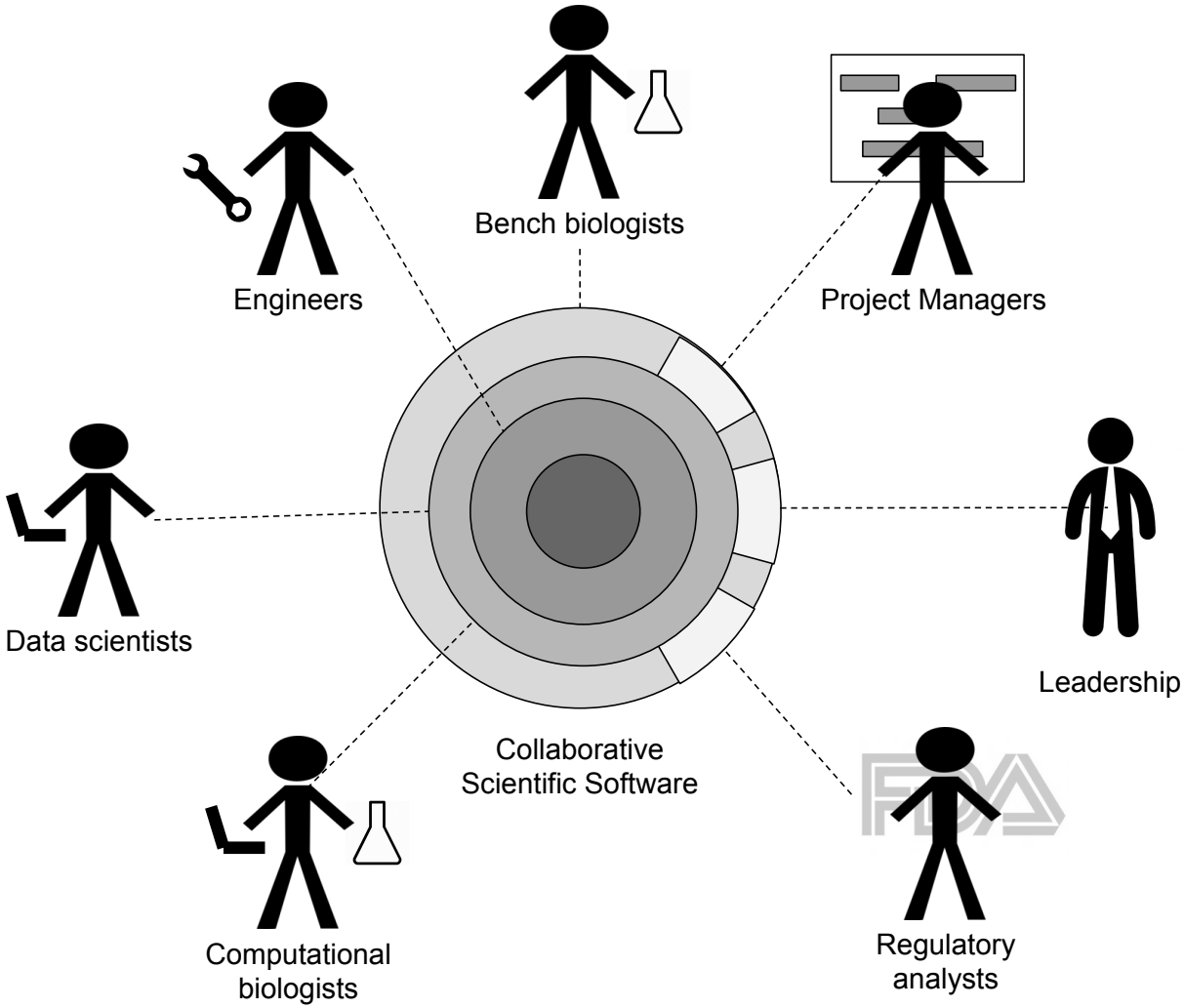
Open-sourcing policy and process

- Decide to open-source early in incubation process
  - Potentially separate open-source and in-house codebases
  - Most infrastructure will need to be open-source, in order to support open-sourcing of dependents
- Piggyback on existing manuscript publication process
  - Code review in place of reviewing text
  - Encourage cross-functional reviews for learning and potential reuse/unification of software
- Develop understanding and standard practices around licensing
- Adopt open-source culture internally (*inner sourcing*)



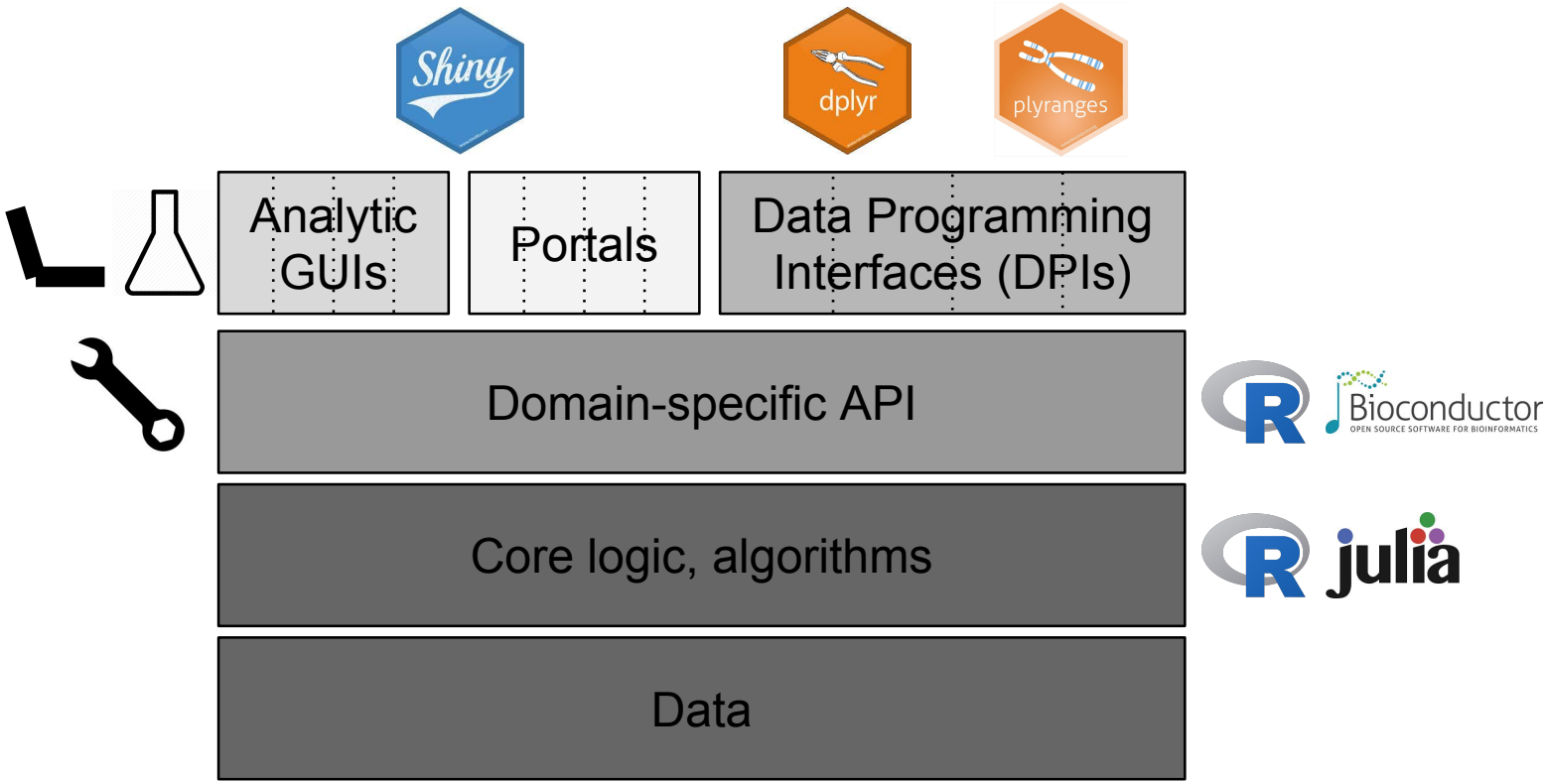
Science is collaborative

so our software should integrate multiple perspectives



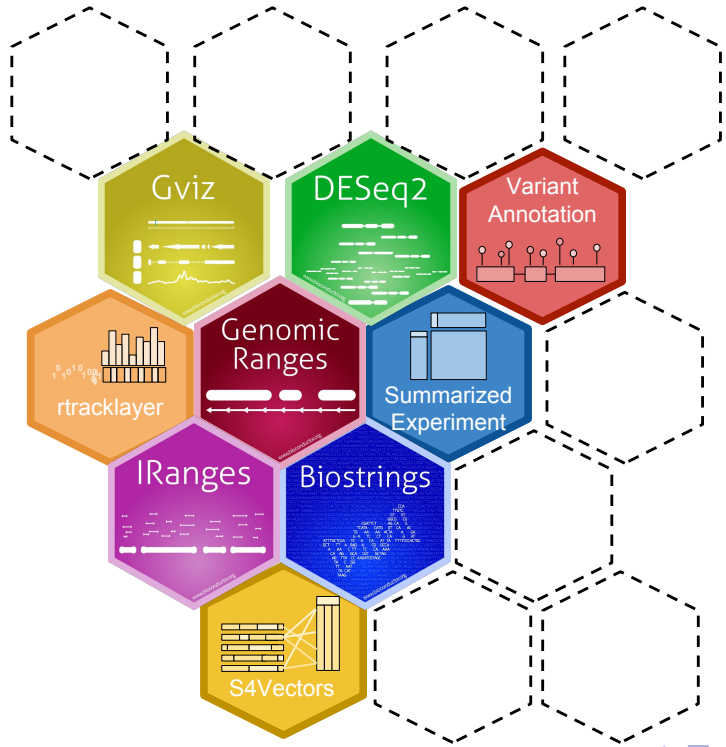
The general scientific software stack

An interface for every role

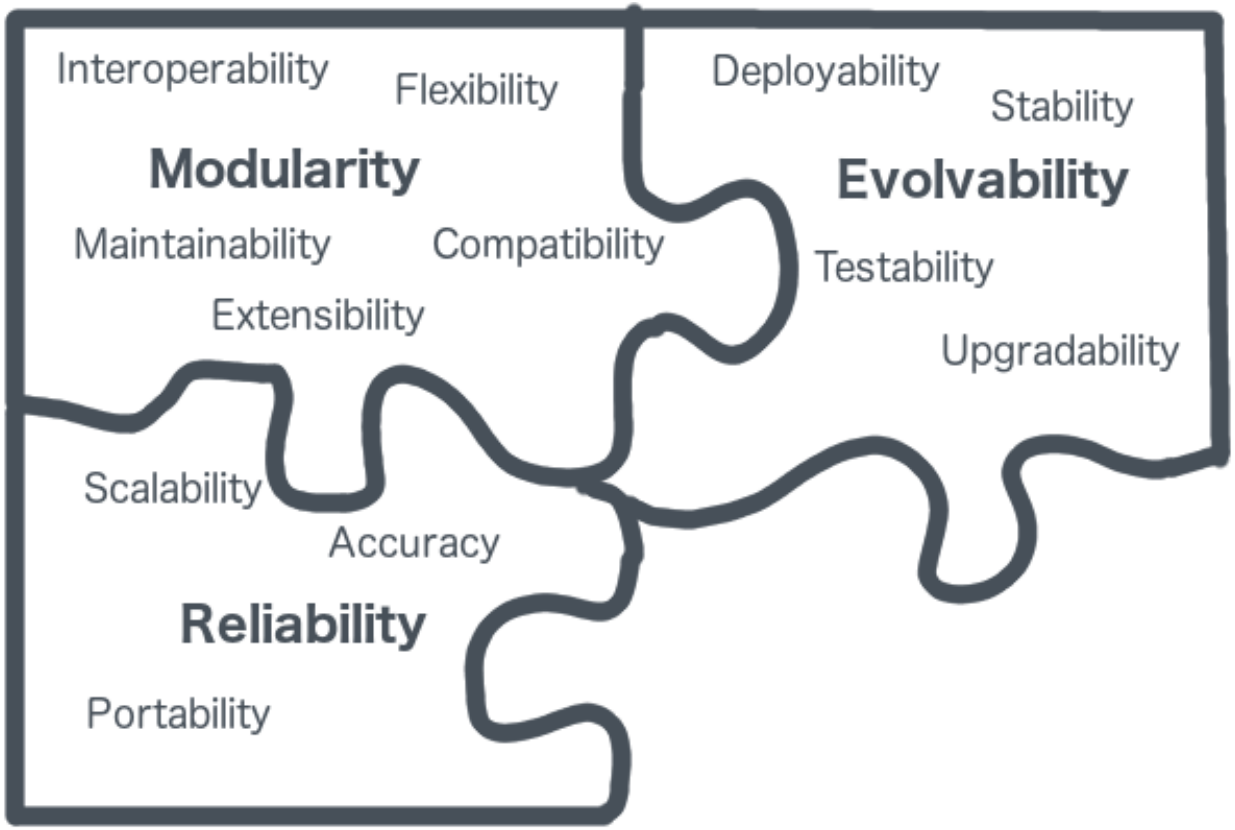


Bioconductor

- Extends R with an integrated platform for exploratory genomics
- Implements standardized, scalable, interoperable data structures
- Hosts state-of-the-art algorithms
- >1500 community-contributed packages



Usability: the missing piece



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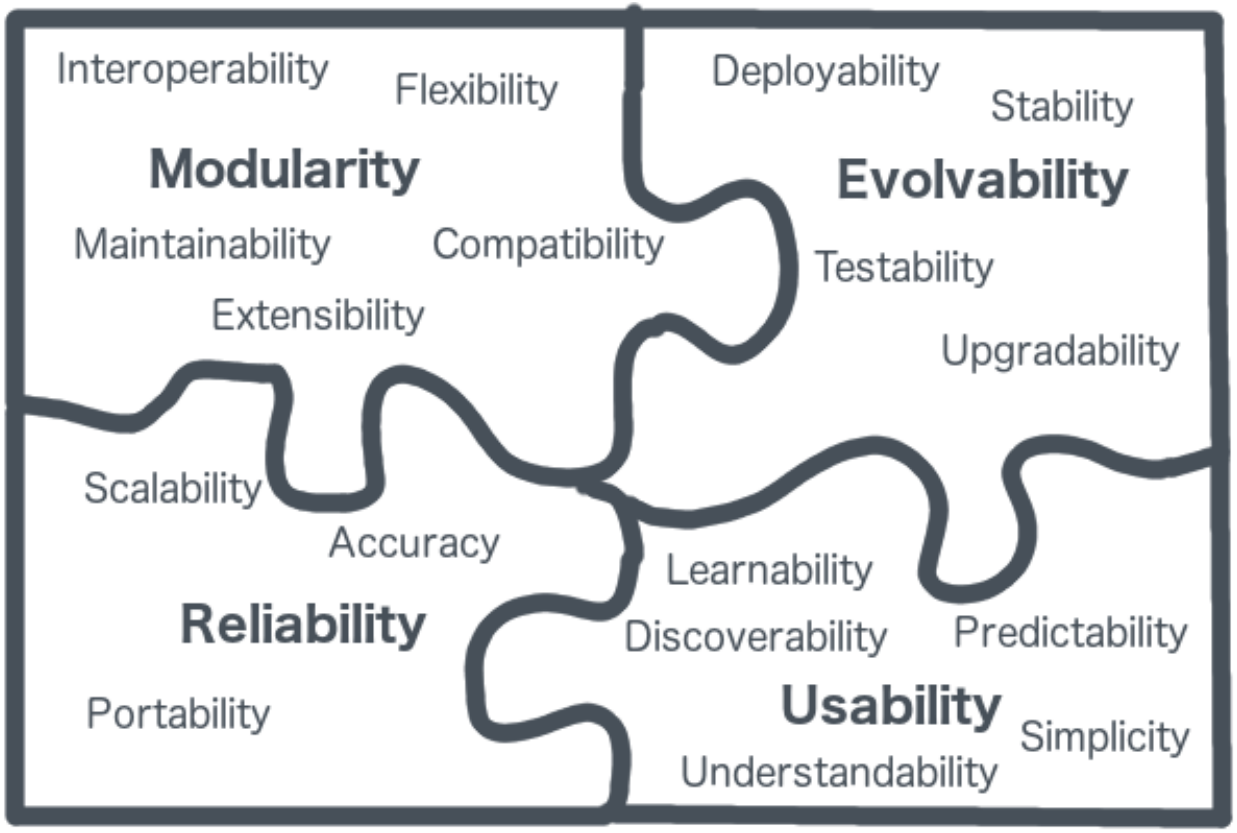
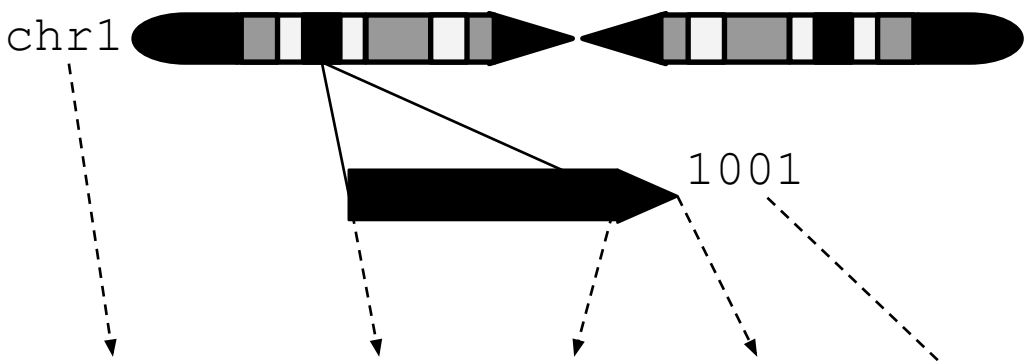


Genomic Ranges



seqname	start	end	strand	gene_id	score
chr1	102012	120303	+	1001	10
chr1	520211	526211	-	2151	25
...	...	...	...	...	...

plyranges: a grammar for genomic data manipulation

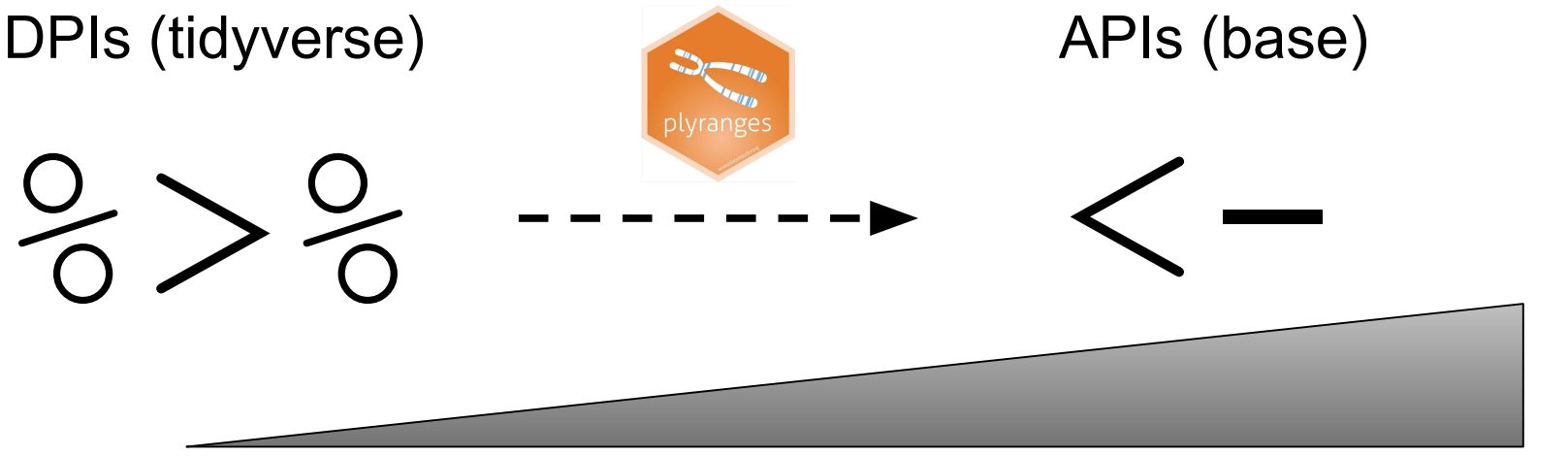
- Extension of relational algebra and dplyr syntax to genomics
- Operations are:
  - Cohesive (do a single thing)
  - Endomorphic (`<T> <? extends T> f(T x)`)
  - Verb-oriented in syntax
- Based core Bioconductor data structures:

  GRanges represents annotated genomic ranges

  SummarizedExperiment coordinates experimental assay data with sample and feature annotations
- Fluency emerges from chaining of verbs

```
compute_coverage("a.bam") %>%
    filter(score > 0) %>%
    intersect(read_bed("b.bed"))
```

Formal data structures enable transition to programming



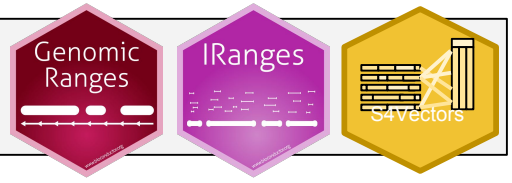
Programming in the **small**
Reusable, functions

Programming in the **medium**
Generalized, documented, tested, OOP, packaged

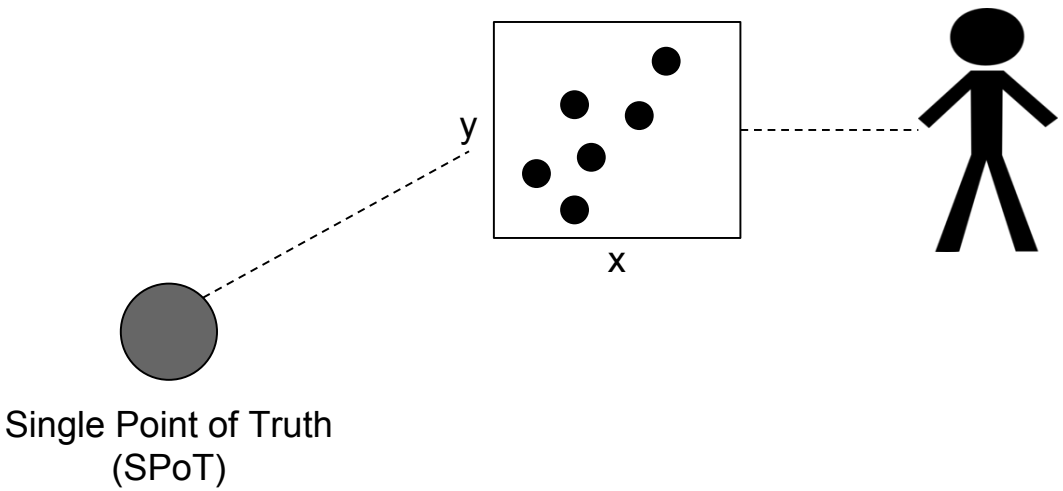
Programming in the **large**
Scalability, heterogeneous architectures, interfaces

Bioconductor
OPEN SOURCE SOFTWARE FOR BIOINFORMATICS

Interoperable data structures



Single points of truth enhance collaboration



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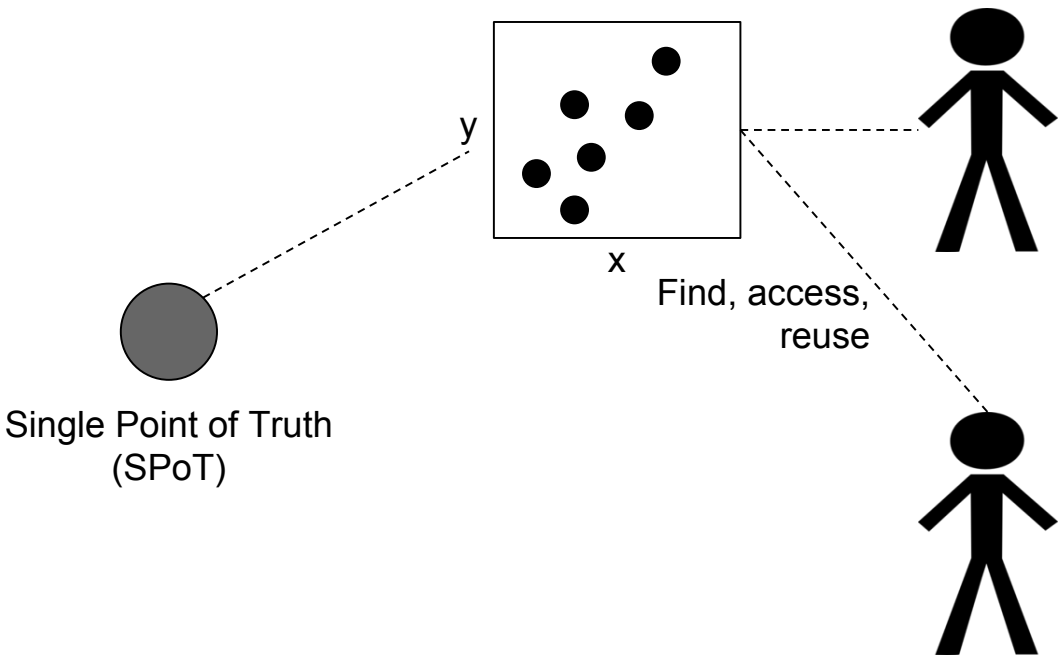

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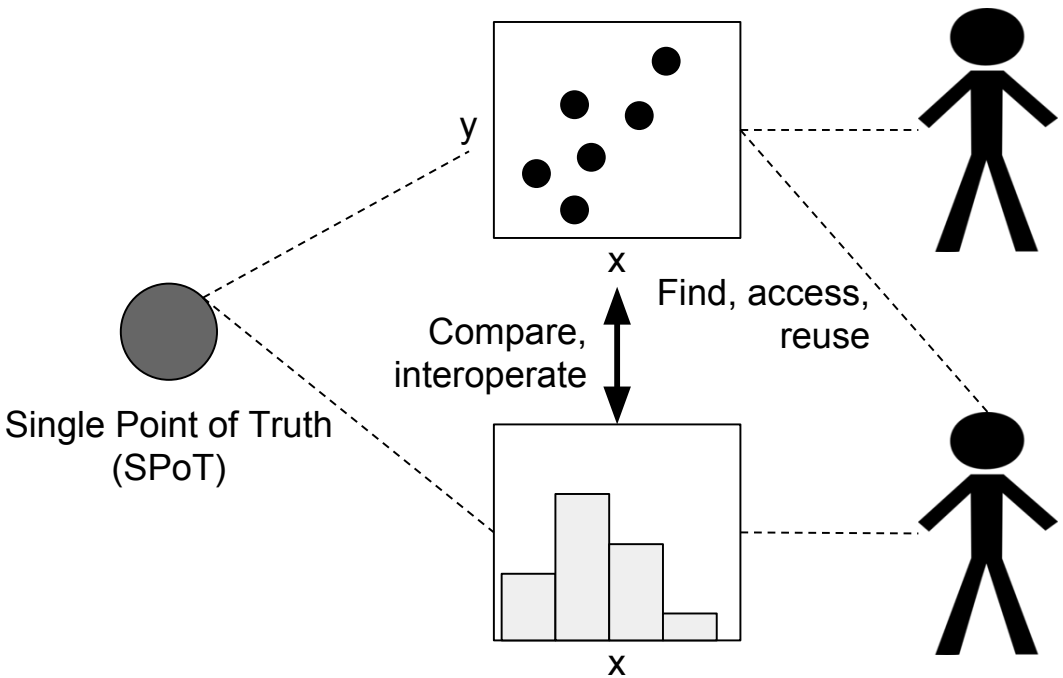

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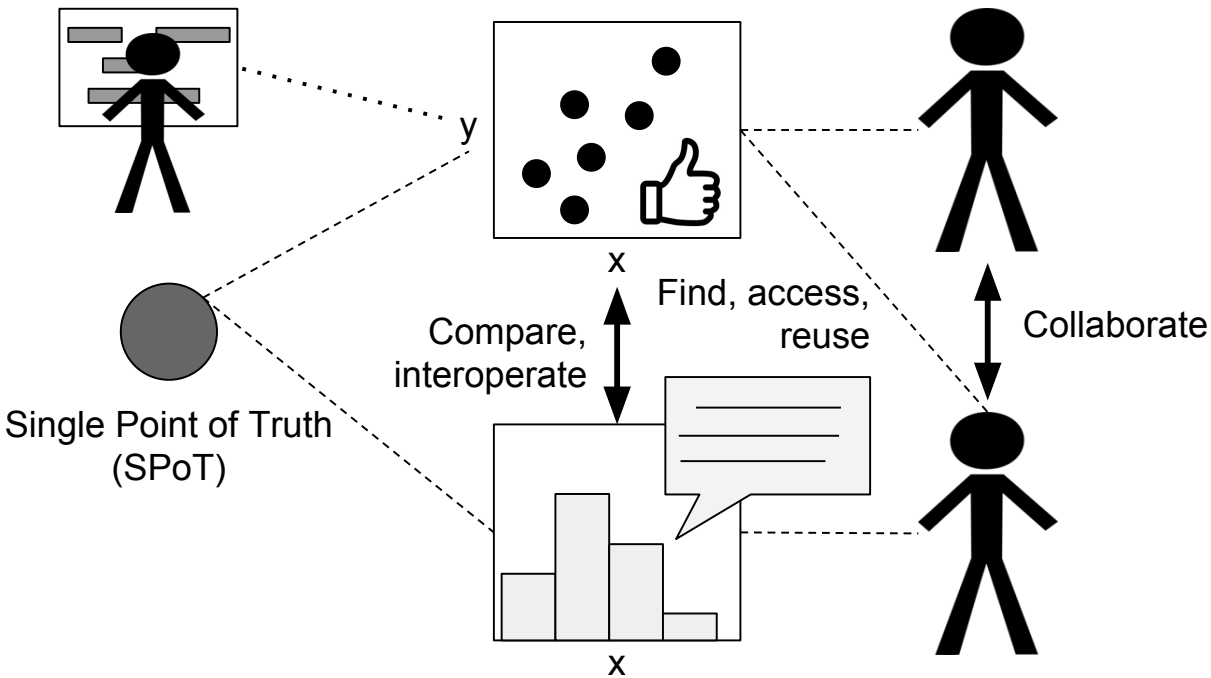

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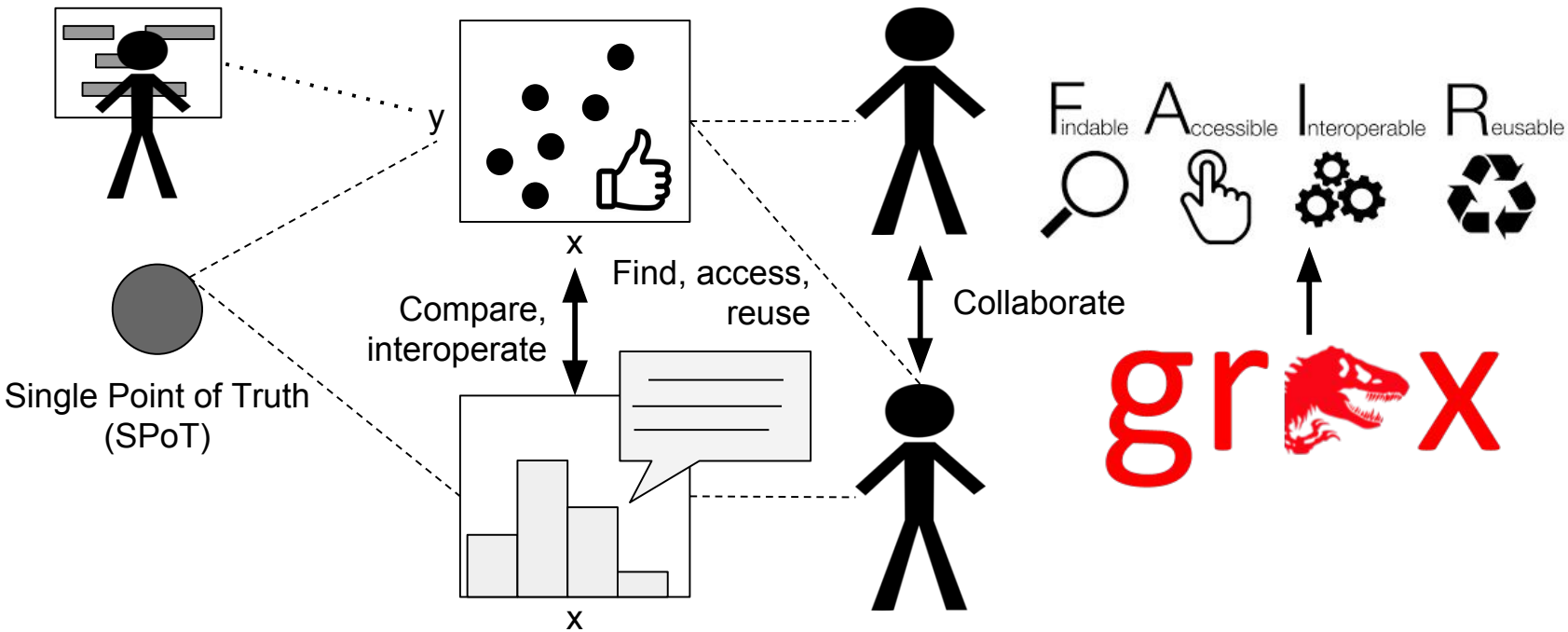
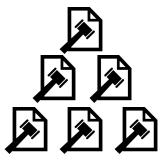


Requirements of a data analysis environment

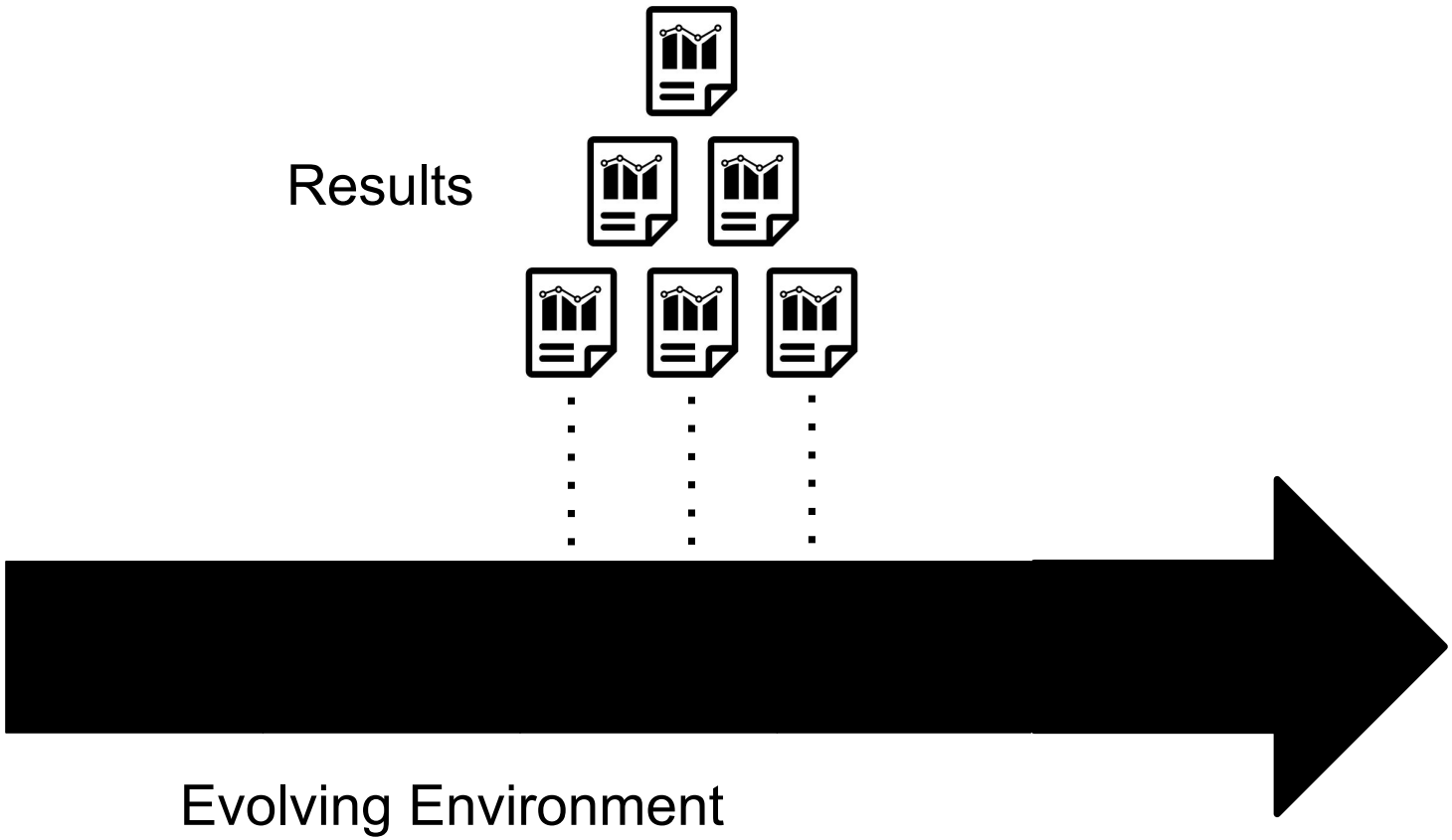
Metered evolution,

- Cohort-based build, test, deploy
- Discover tools and applications

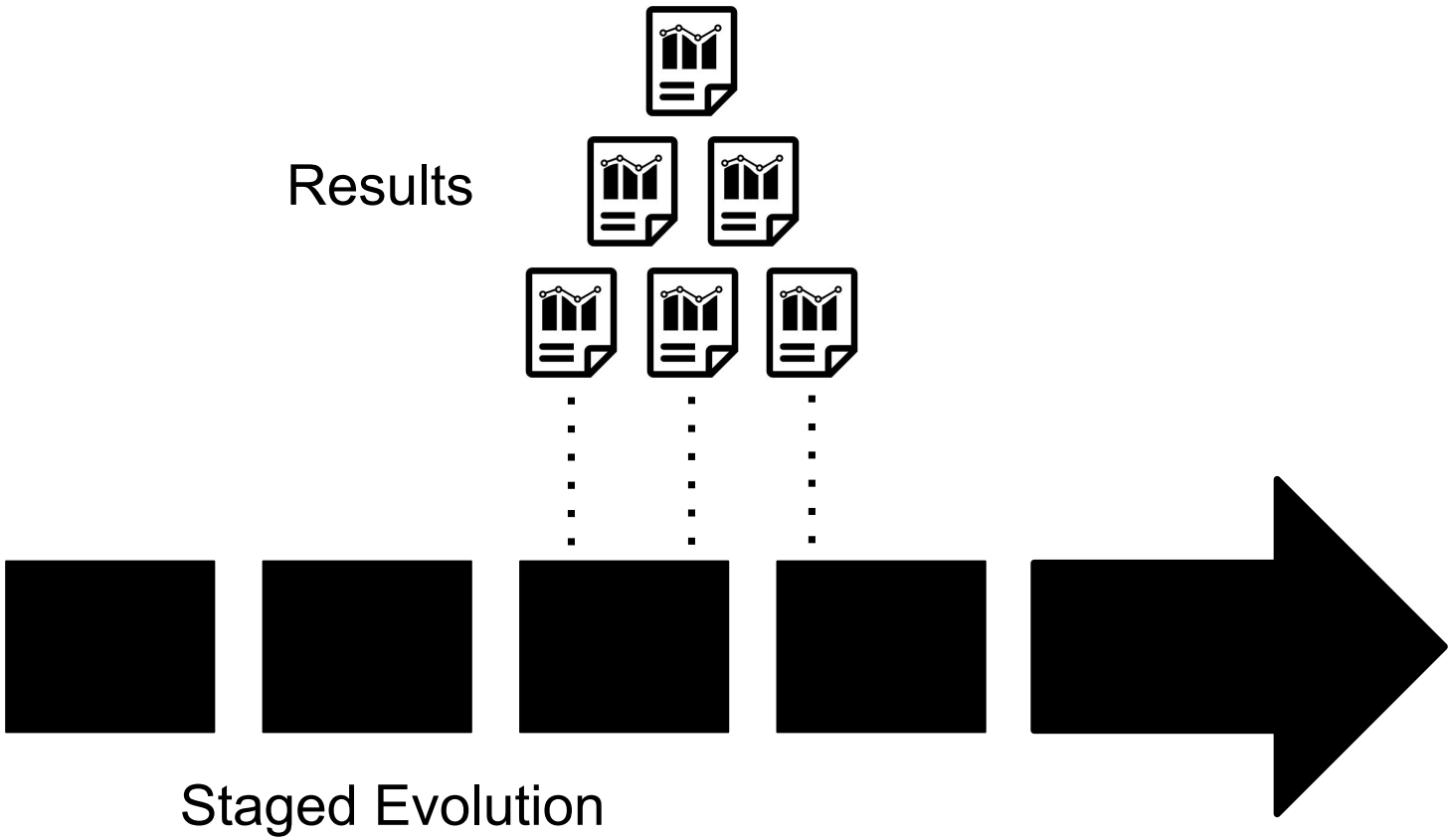


Stratified specialization across groups,

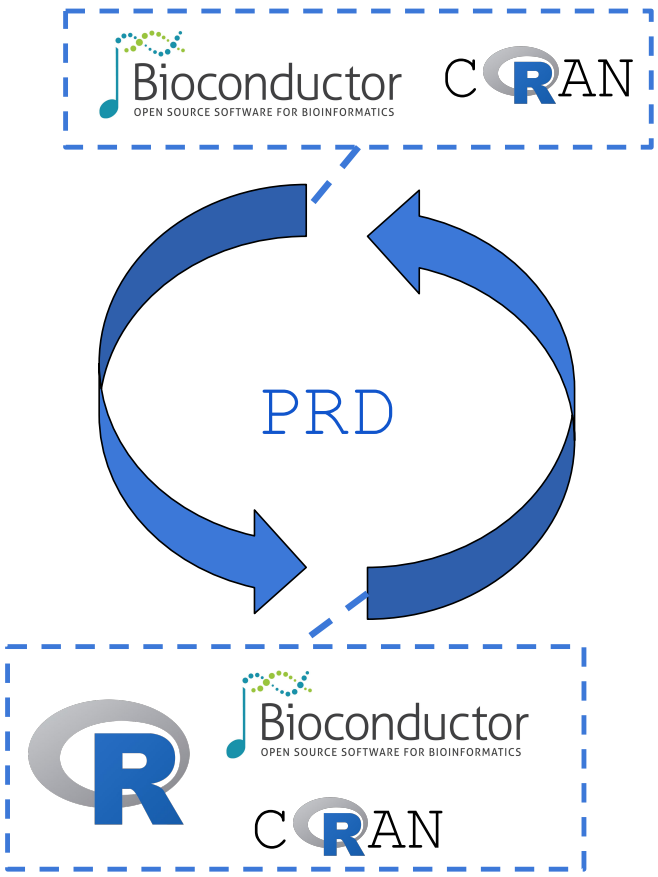
Metered evolution



Metered evolution



Graded evolutionary policies



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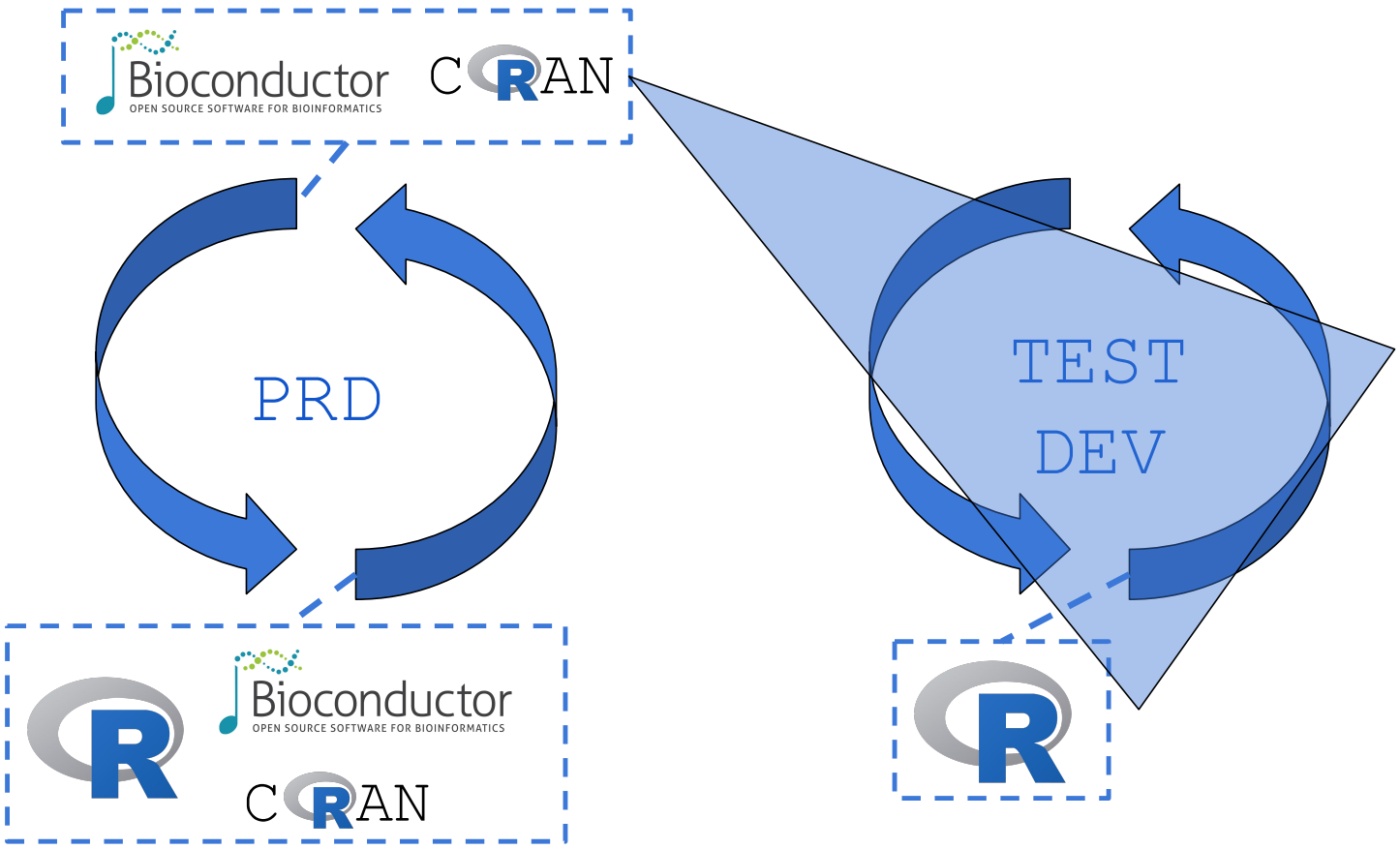
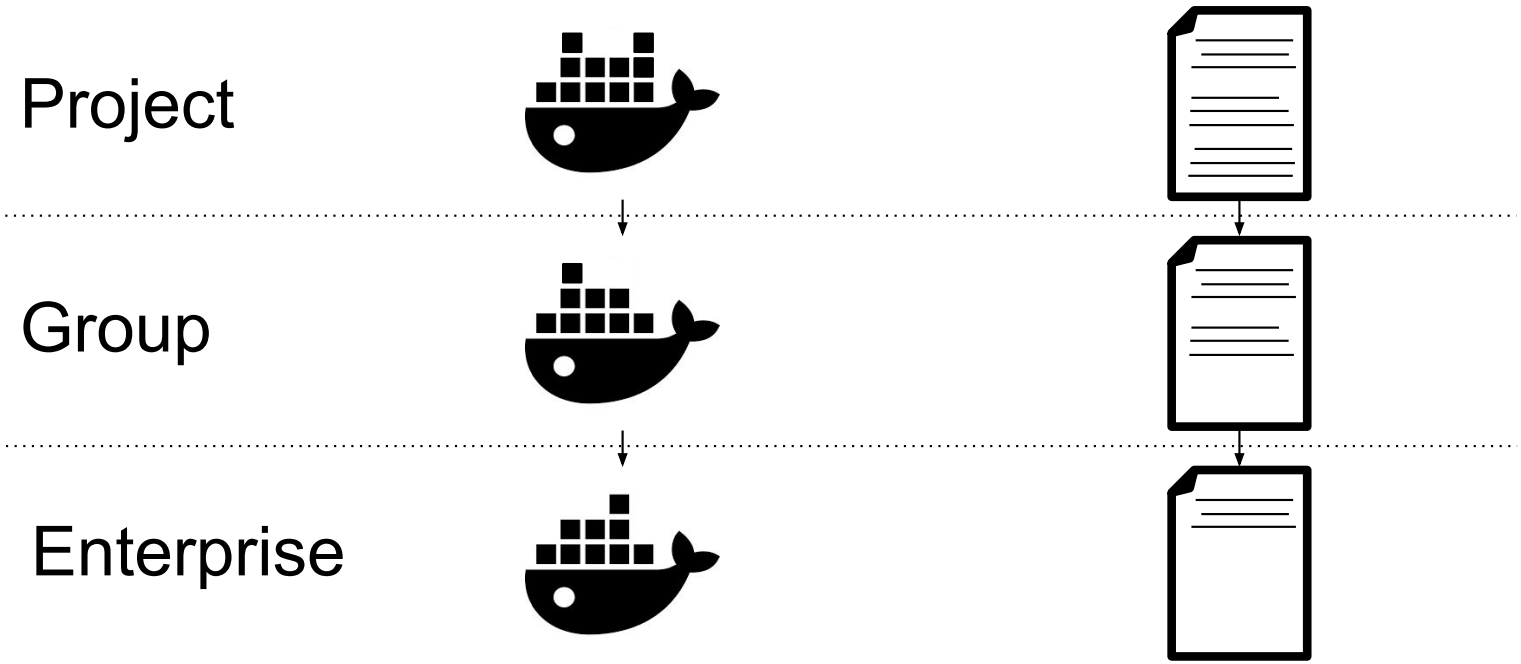
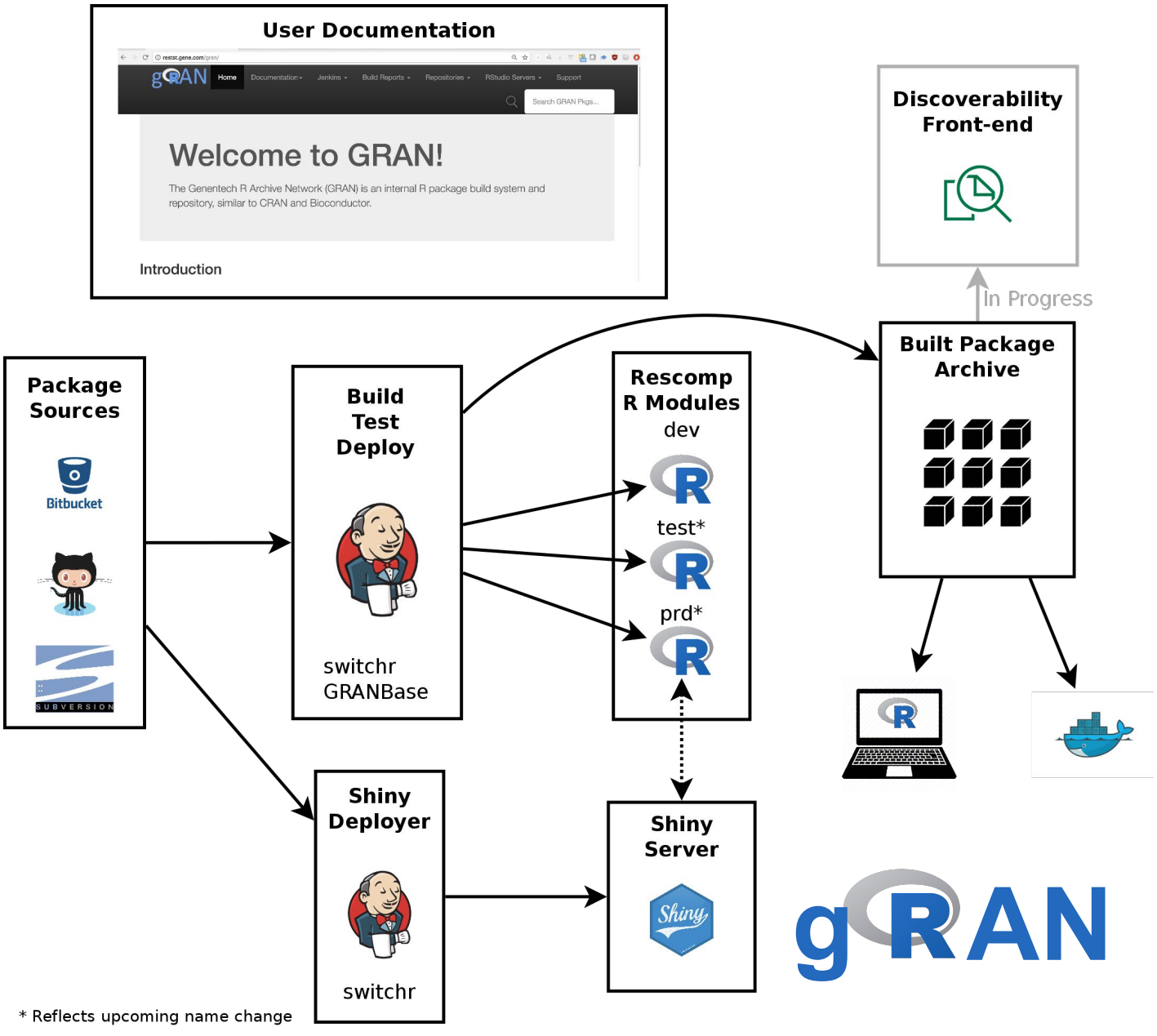


Stratified specialization



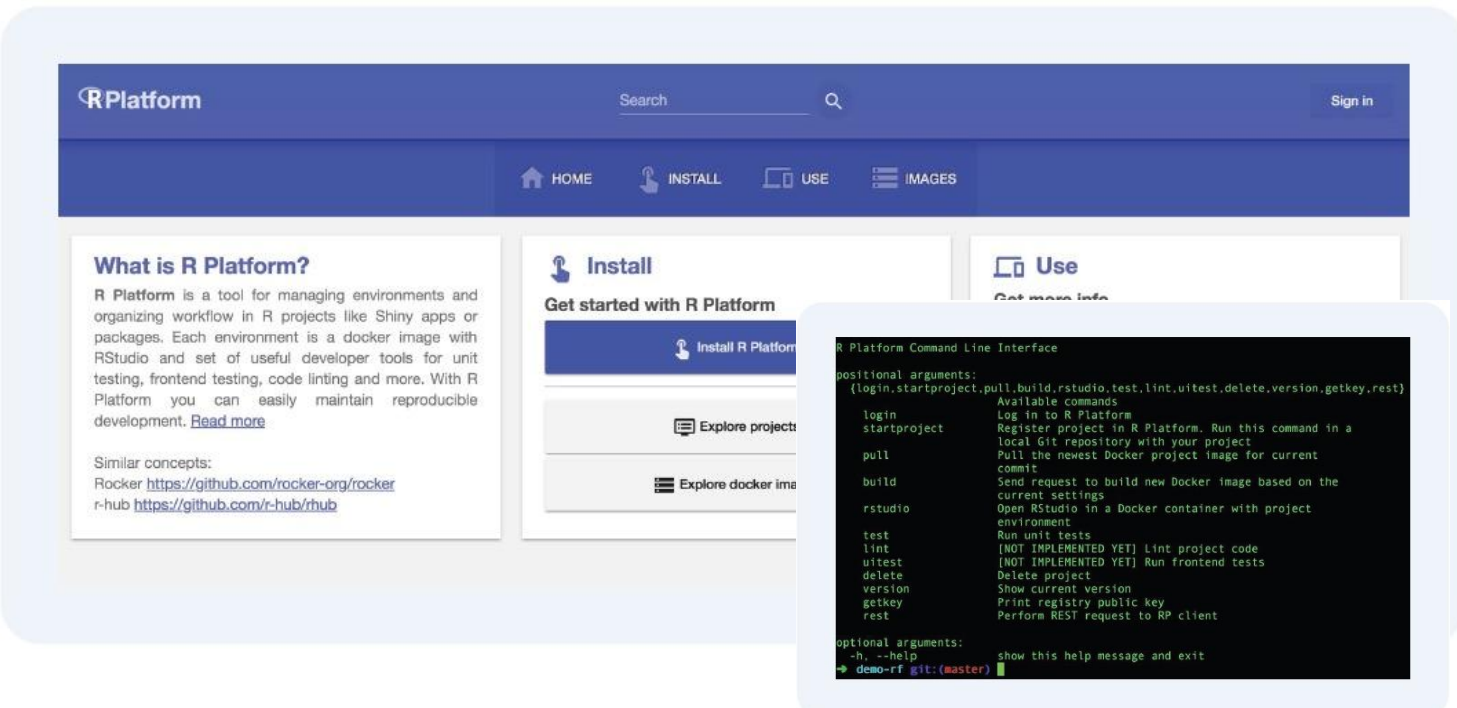
Environment orchestration (Gabe Becker)



Rapid deployment with the *R Platform*

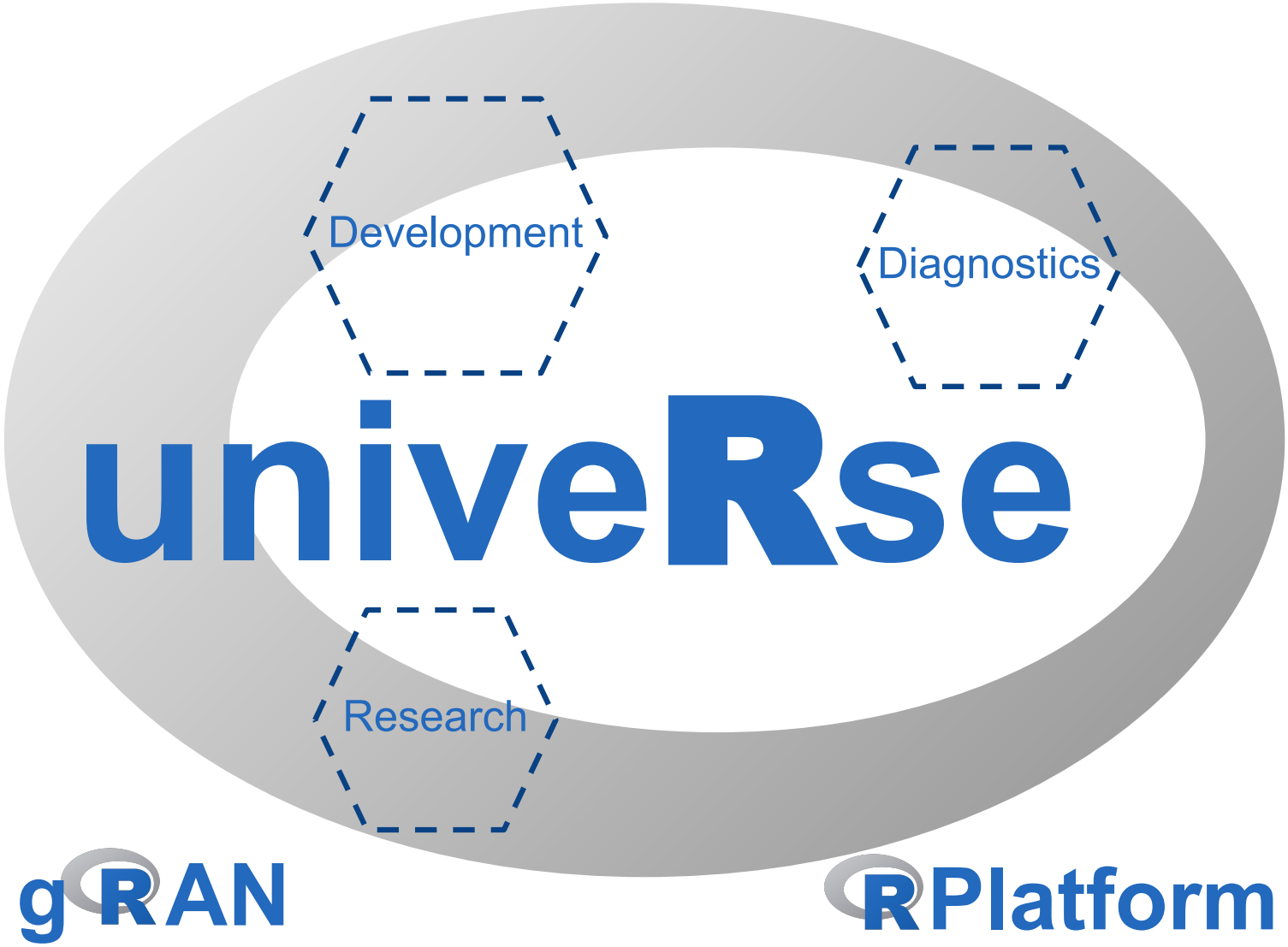
Dariusz Ratman, et al.

- The R Platform provides agile deployment of project-specific development and analytical environments through containers
- Automatic generation of Docker containers from R packages
- Share containers through an internal registry
- Automatic continuous integration and testing in multiple environments

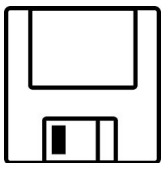


The Roche R Universe

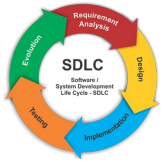
with Reinhold Koch, Sebastian Wolf, Gabe Becker



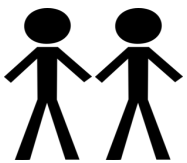
Summary



Leveraging R means becoming a software company



The software incubator translates scientist innovations into reliable software



Scientific software is challenged to enable active collaboration

gRAN

Multi-layered and strategically evolving environments can unify scientific computing across the enterprise