

Explorable Labs

RDKit microservices

Why and how to automate compute-intensive applications

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Flexibility is key!

Different teams have different needs.

Frontend trends change quickly.
(Jupyter, Retool... what's next?)



Admin Explorable Labs 12:45 PM
CN1C=NC2=C1C(=O)N(C(=O)N2)C

chemdata APP 12:45 PM
ExactMolWt: 194.08037556
FpDensityMorgan1: 1.1428571428571428
FpDensityMorgan2: 1.7857142857142858
FpDensityMorgan3: 2.4285714285714284
HeavyAtomMolWt: 184.11399999999998
MaxAbsPartialCharge: 0.3317034326359889
MaxPartialCharge: 0.3317034326359889
MinAbsPartialCharge: 0.3278634660994821
MinPartialCharge: -0.3278634660994821
MolWt: 194.194
NumRadicalElectrons: 0
NumValenceElectrons: 74

But if your key computational tools exist on cloud API endpoints, they easily integrate into new frontend tools. API = modular.

You can use managed microservices if needed. (E.g. Serverless or Stdlib for lightweight Lambda tasks, Explorable Labs for Fargate!)
Many proprietary tools offer APIs already.

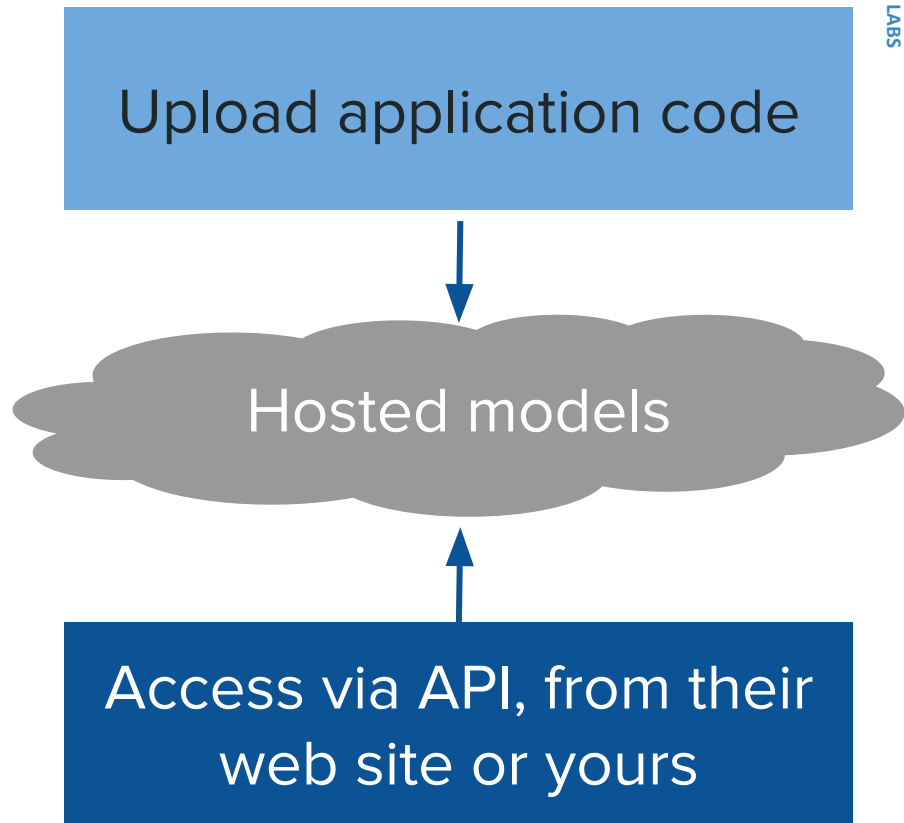
https://github.com/explorablelabs/rdkit_api

Why use microservices instead of reserved instances or local infrastructure?

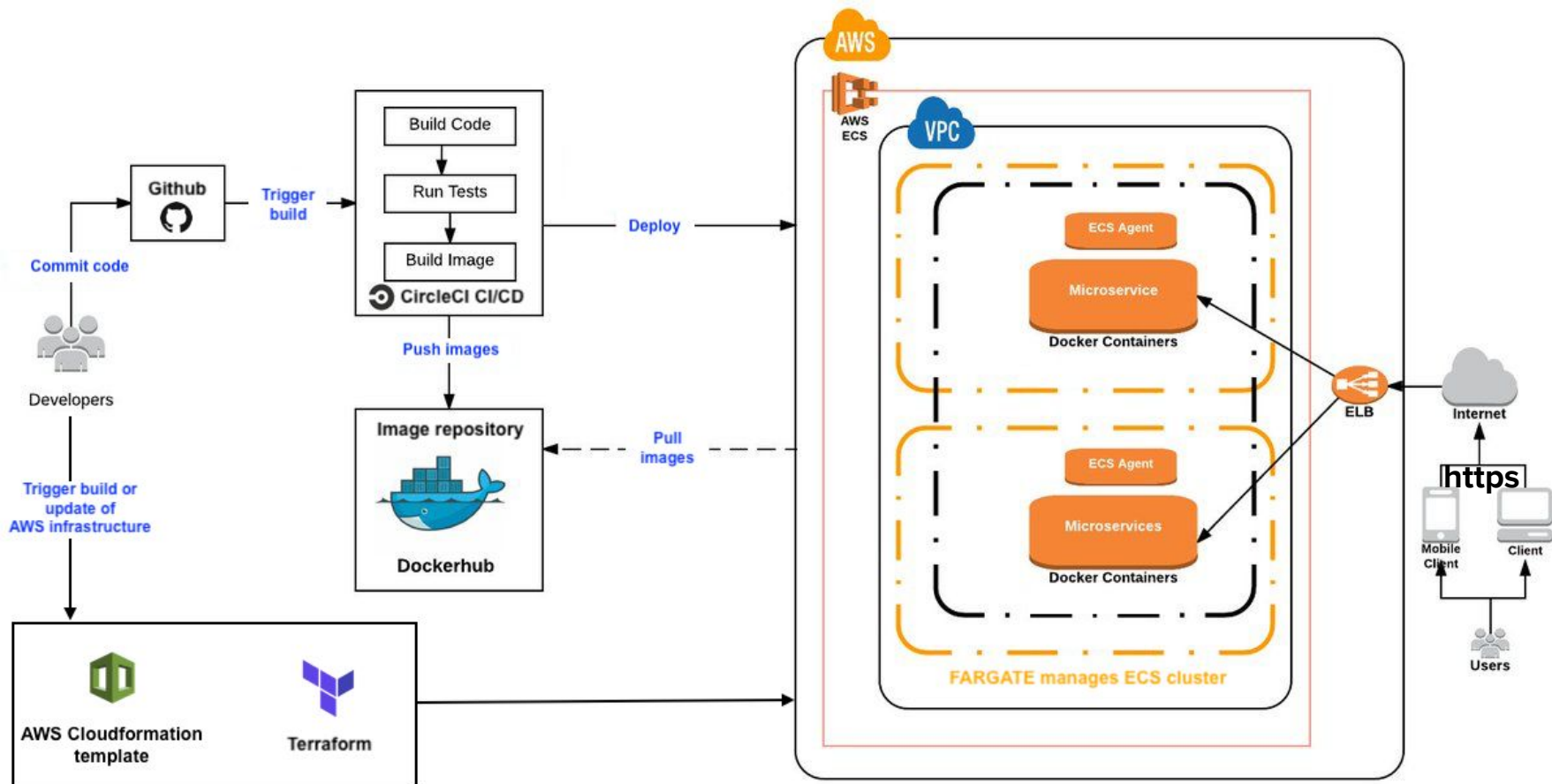
It's cheaper, more reliable, and more secure!

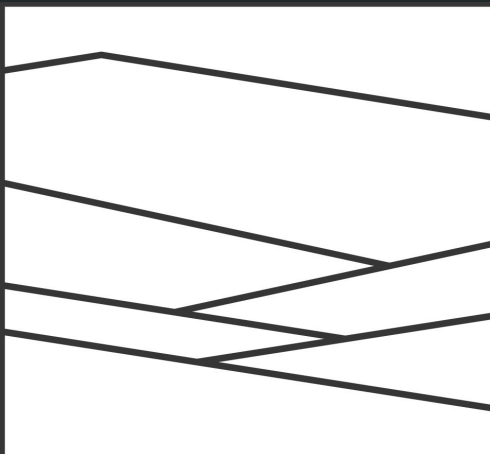
Costs scale with compute time
(breakeven is around 70% usage of
a reserved instance)

The cloud provider handles server
maintenance and patching. If
needed, a new microVM is spun up
in <125ms (!!)



DIY API Architecture





Hosted compute-intensive applications

Explorable Labs

We help computational scientists scale
their work in the cloud.

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