

Software containers and reproducibility: what can IVOA learn from it?

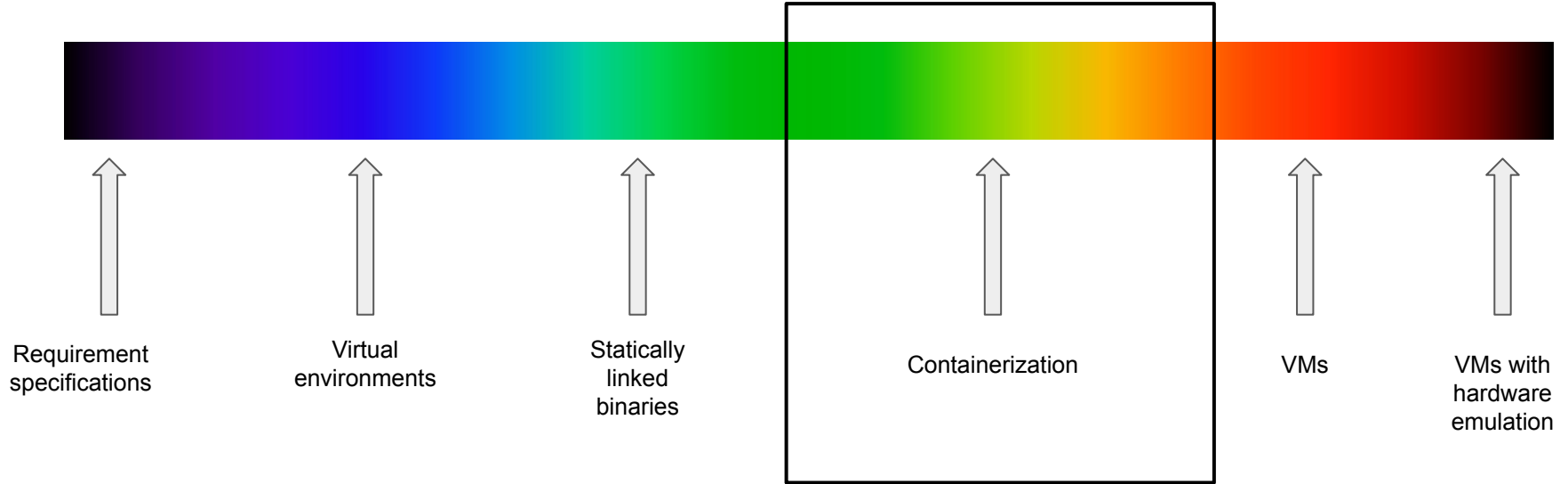
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The dependency hell

- How to compile a software?
- How to set up a software?
- How to reproduce a run?

Solutions spectrum



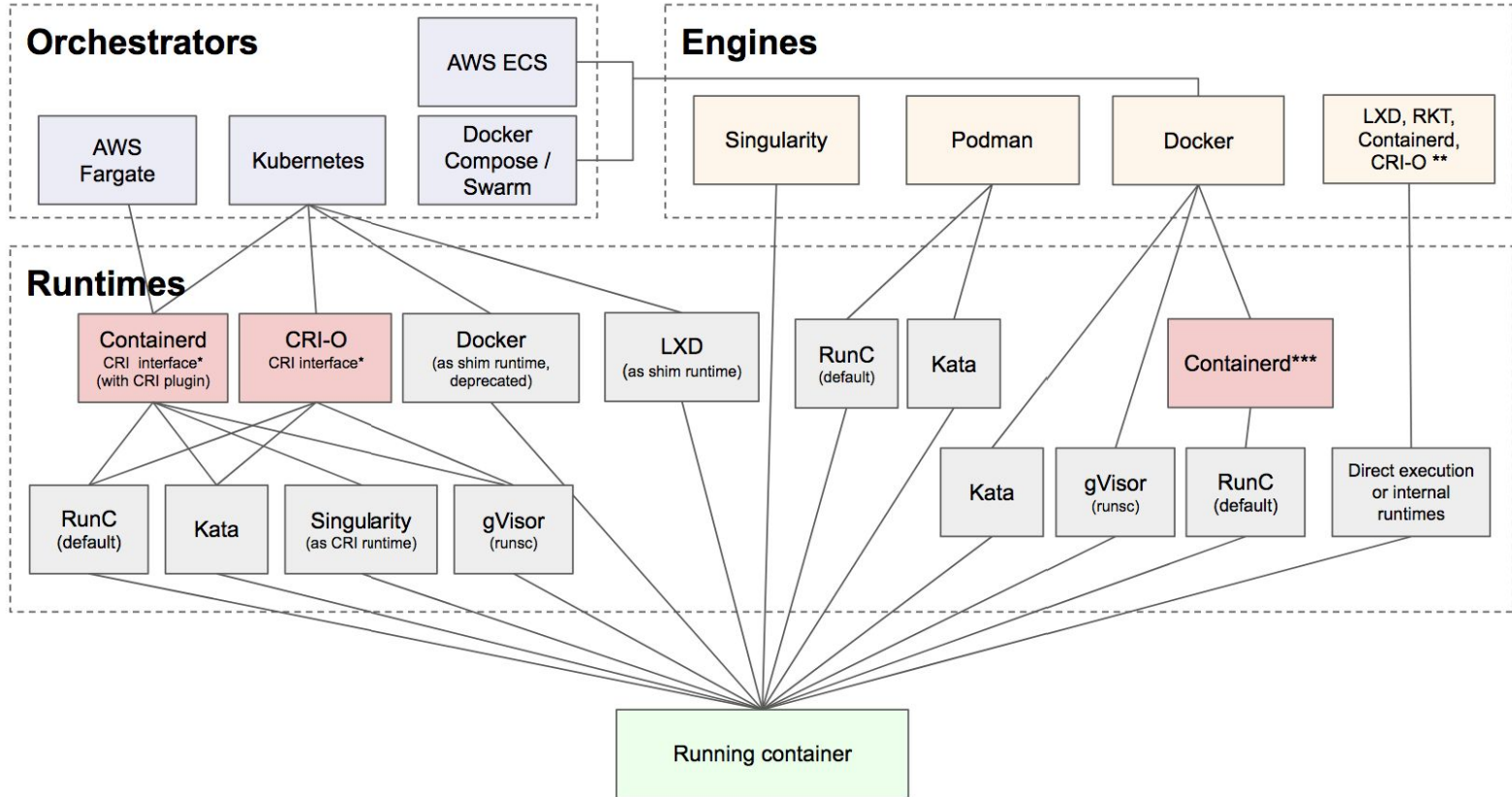
Software containers

“A container image is a lightweight, standalone, executable package of software that includes everything needed to run an application: code, runtime, system tools, system libraries and settings.”

Open Container Initiative standards:

- Images (incremental FS bundles)
- Registries and manifests
- Runtimes (hi and low level)

Containerisation landscape



The definitive(-ish) solution for reproducibility

- All dependencies always carried with the container
- Multi-OS and multi-architecture support
- Engines and runtimes for every need
 - Rootful
 - Root-less
 - With Kernel virtualisation
 - With HW virtualisation and emulation
 - *which are basically VMs, but with all the containerisation ecosystem benefits*

But wait.. where is all the complexity gone?



Hidden complexity

- Multiple architectures and OSes → multiple images per tag!
- Docker desktop (Mac/Win) does HW emulation if working with non-native architectures
 - *and crashes with instruction set-optimized executables, i.e. Chrome*
- Rootful, rootless, virtualisation etc. bring unexpected incompatibilities
 - *limitations, UIDs/GIDs, file permissions, PIDs, networking...*
- Container registries with private containers still hard to support
- Drop-in replacements (i.e. Podman, Kata) are such until they are not
- Creating truly re-buildable Dockerfiles requires good craftsmanship
- Kernel-level optimisation basically do not fit with the “build once, run everywhere”

Takeaways

- Software containers are in general very good for reproducibility
- Lot of complexity was hidden but is re-arising
 - *Apple Silicon didn't help*
- Some early days, naive choices are basically design flaws
 - *will be hard to eradicate*
- An informed, educated usage can solve the majority of the issues

Thank you!