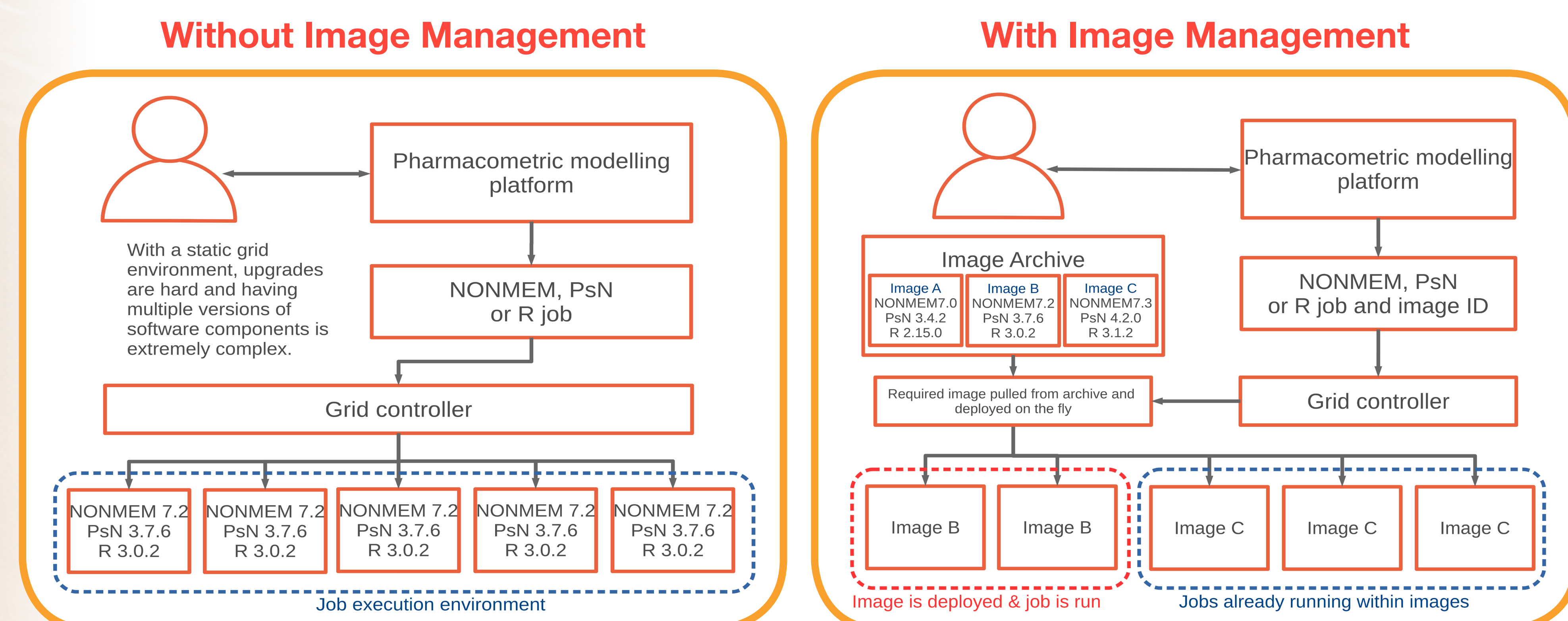


Reproducible Analysis Environments for Pharmacometric Modelling and Simulation

Objectives: To provide an easily reproducible analytical computing environment for pharmacometric modelling and simulation without compromising the speed with which a computational environment can be deployed.

Methods: A suite of common tools such as NONMEM, PsN, R etc. are installed with an operating system and a suite of validation tools, inside an 'image'. The word 'Image' is used to describe a complete description of a working environment, for deployment onto your computing infrastructure. This may be a Virtual Machine, a docker container, or a cloud provider image such as an Amazon Machine Image. The validation tools are made available for running on a scheduled or ad-hoc basis and the final image is validated using these tools before deployment. When a new version of a software component is released, a new version of the image is created. When an image reaches the end of its useful life, for example, if it contains an obsolete piece of software, that image is retired and added to an archive for future use. Any given analysis has the image used recorded against it.

Results: As the results of past analyses are tied to a particular image, we found it simple to run a given analysis again, on the same image. Over time, a library of images is created and archived. This allows an organisation to effectively go 'back in time' with their analysis environments should a query be made against an earlier analysis. Using the ad-hoc validation tools we demonstrated that it is possible to perform immediate validation of any image deployed from the archive. This provides the user and regulators with assurance that the resulting output of analyses performed using that image are as expected and consistent with any analysis run previously.



Conclusions: We proved that the ability to version control validated analysis environments is a compelling benefit for anyone engaged in pharmacometric computing. We found this to be particularly true where such work is heavily regulated and the ability to quickly and easily re-run an old analysis in a validated manner is essential. Further, we demonstrated that keeping track of the 'library of images' can be difficult and should therefore form part of the overall pharmacometric platform in use. The flexibility provided by such an approach is highly desirable as it frees your compute infrastructure from being a single purpose environment to being able to perform multiple analysis duties using whatever tools are appropriate.