# Infrastructure for Efficient and Effective Implementation of Modeling and Simulation in the Cloud

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# History of Metrum Infrastructure

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GRID ENGINE

amazon web services™ | EC2

**MOSIX: A Cluster Load-Balancing Solution for Linux**

May 01, 2001 By Ibrahim F. Haddad and Evangeline Paquin

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in Software

*Ibrahim introduces the MOSIX software package and describes how it was installed on an experimental Linux cluster in the Ericsson Systems Research Lab in Montréal.*

Software clustering technologies have been evolving for the past few years and are currently gaining a lot of momentum for several reasons. These reasons include the benefits of deploying commodity, off-the-shelf hardware (high-power PCs at low prices), using inexpensive high-speed networking such as fast Ethernet, as well as the resulting benefits of using Linux. Linux appears to be an excellent choice for its robust kernel, the flexibility it offers, the various networking features it supports and the early availability of its IP releases.


From Issue #85 May 2001

1994 2002 2004 2008 2010 2015

# Infrastructure Requirements

- One stop shop for all tools necessary for Modeling and Simulation
- Qualified, reproducible, and secure environment
- Scalable to meet needs of scientist(s)
- Easily transition from modeling -> simulation -> presentation -> reporting
- Supports multiple areas – PMx, Stats, Systems Pharmacology, Data Science

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*Easy, Agile, Reliable Solution for*

# Big Computation in the Cloud

A product of original R&D
by

METRUM
RESEARCH GROUP

# What is METWORX™?

Browser-based portal to AWS cloud computing

Cloud-powered decision making tools

On-demand

Secure

Autoscaling

Qualified, managed, reproducible

Size-as-you-go encrypted storage

Platform tools include: Rstudio, Perl-speaks-NONMEM (PsN), metrumrg, OpenGrid Scheduler, NONMEM®, OpenBUGS, Stan, Monolix, Matlab, SAS, Pirana Desktop



metworx

*your high-performance platform*

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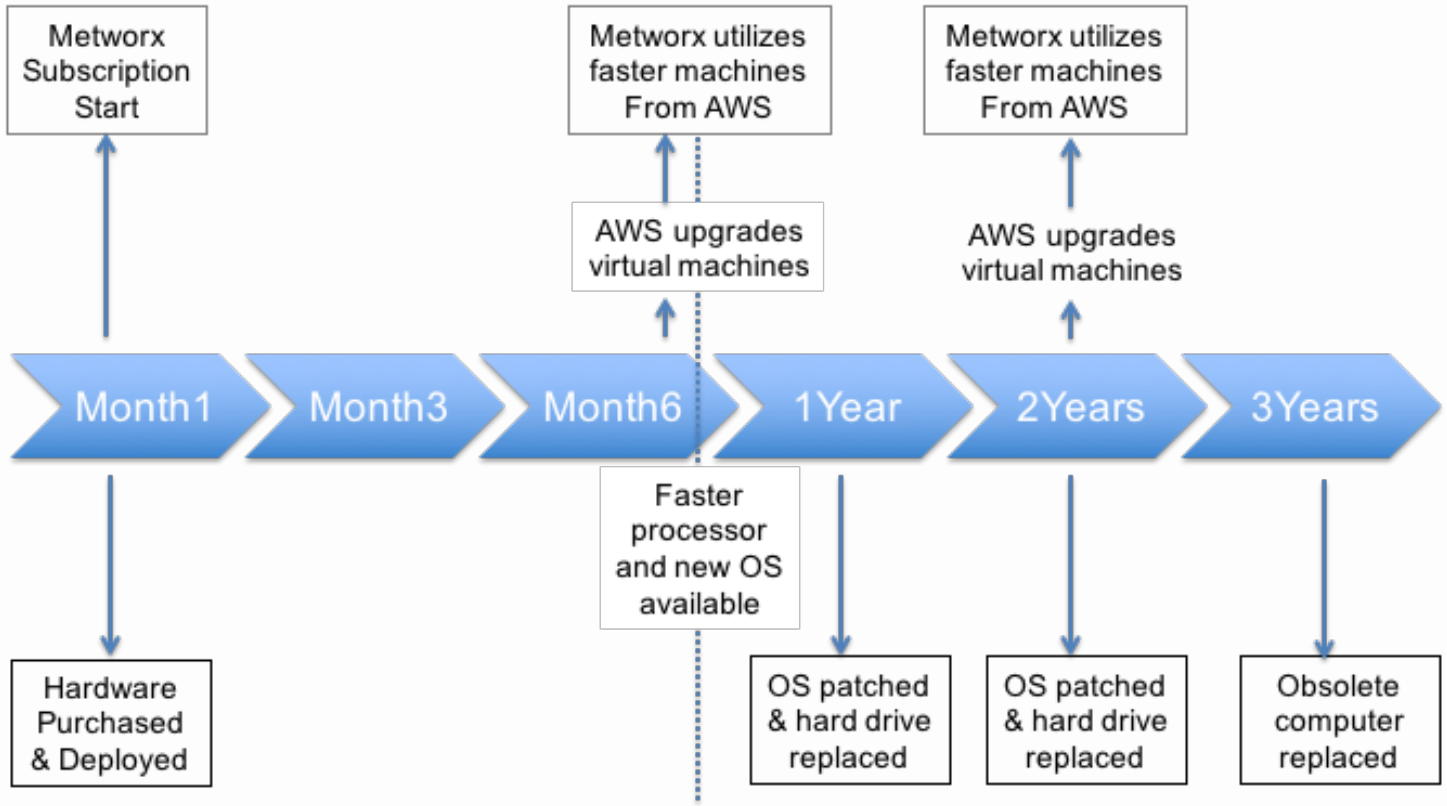
# Cloud vs. Fixed Hardware Investment
## efficient utilization of resources




- Fixed grid becomes obsolete within a year of purchase but must still be maintained until a replacement system is justified.
- Repeated system maintenance cycles result in repeated system down-time.

# Infrastructure in the Cloud

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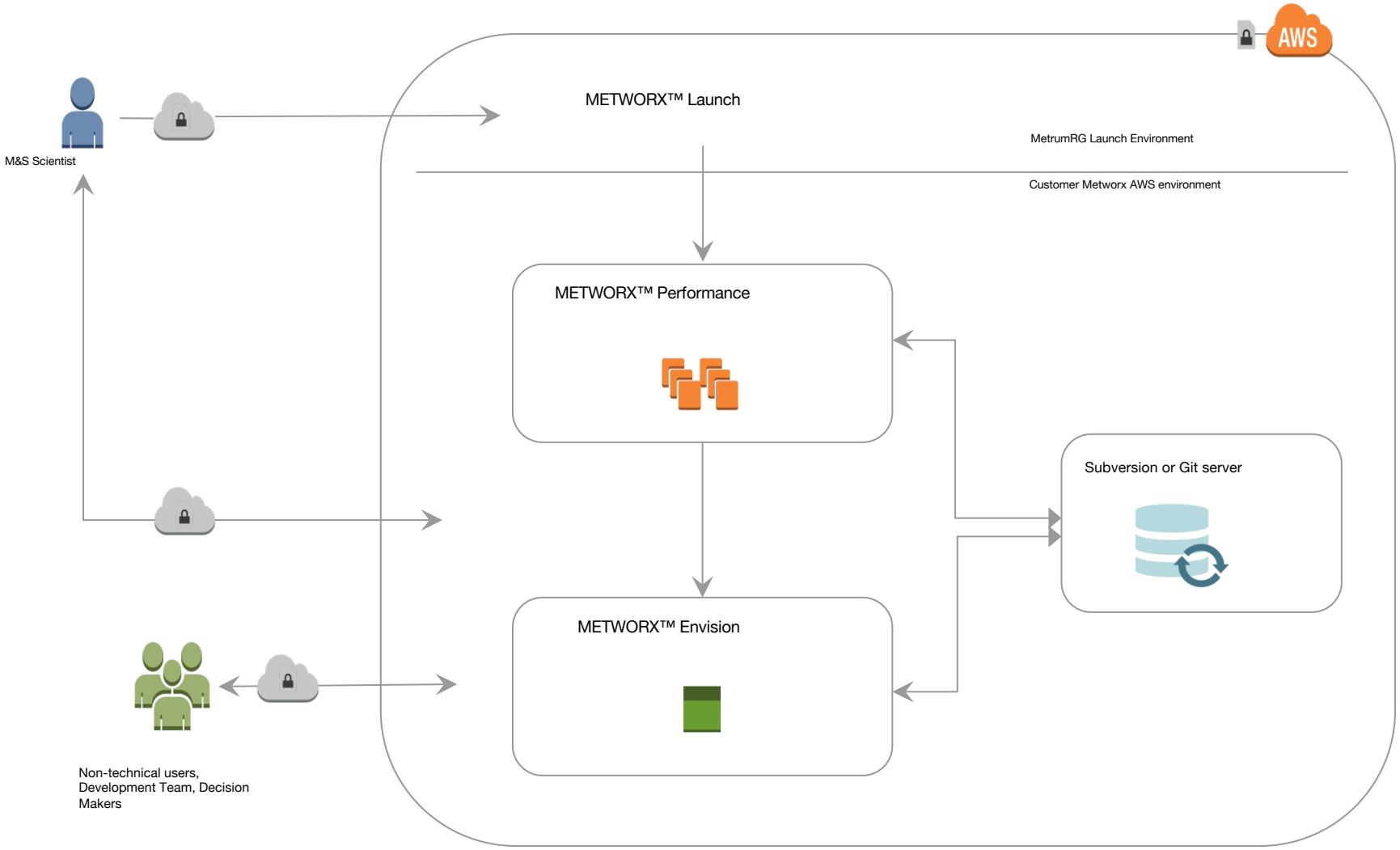
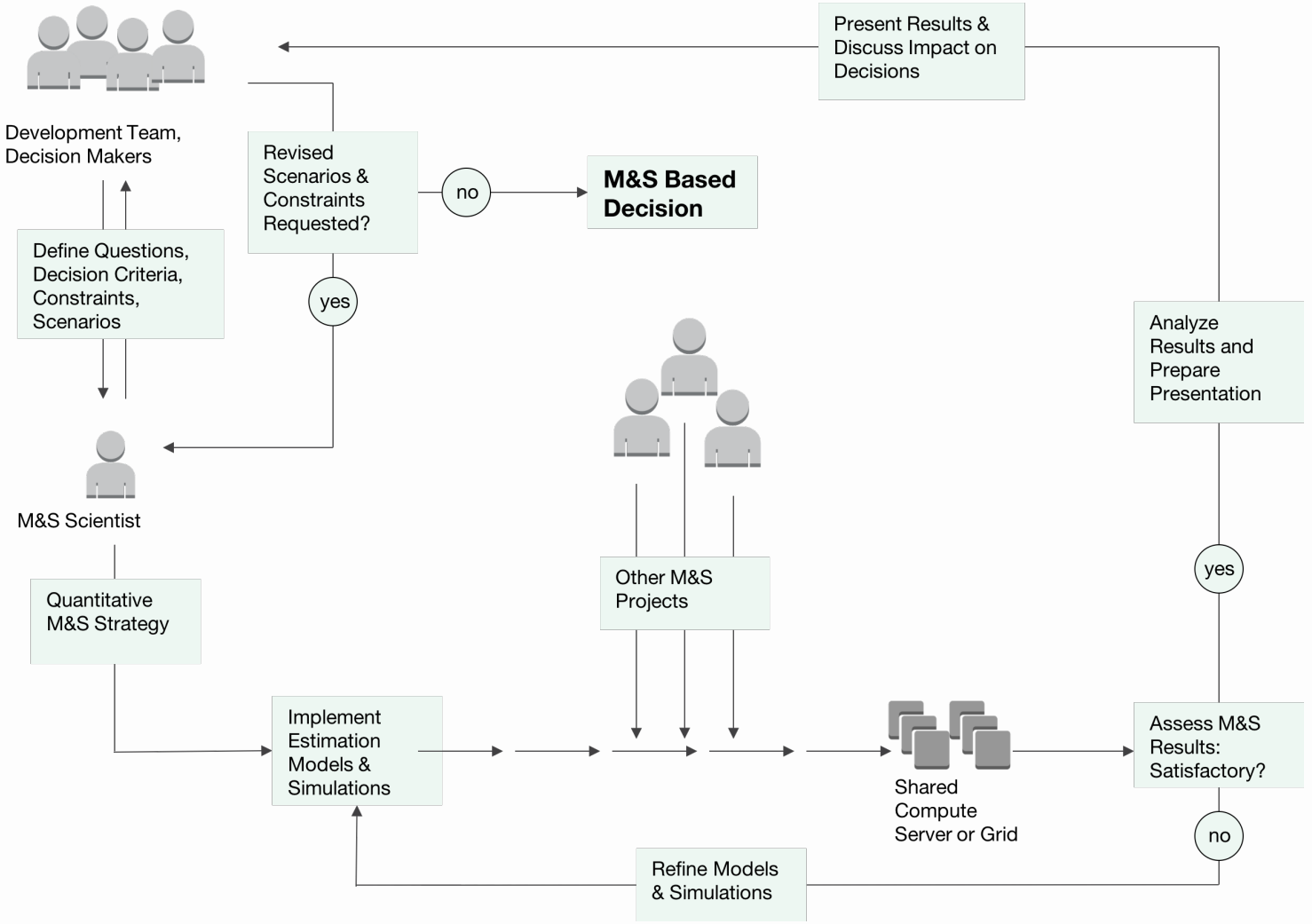
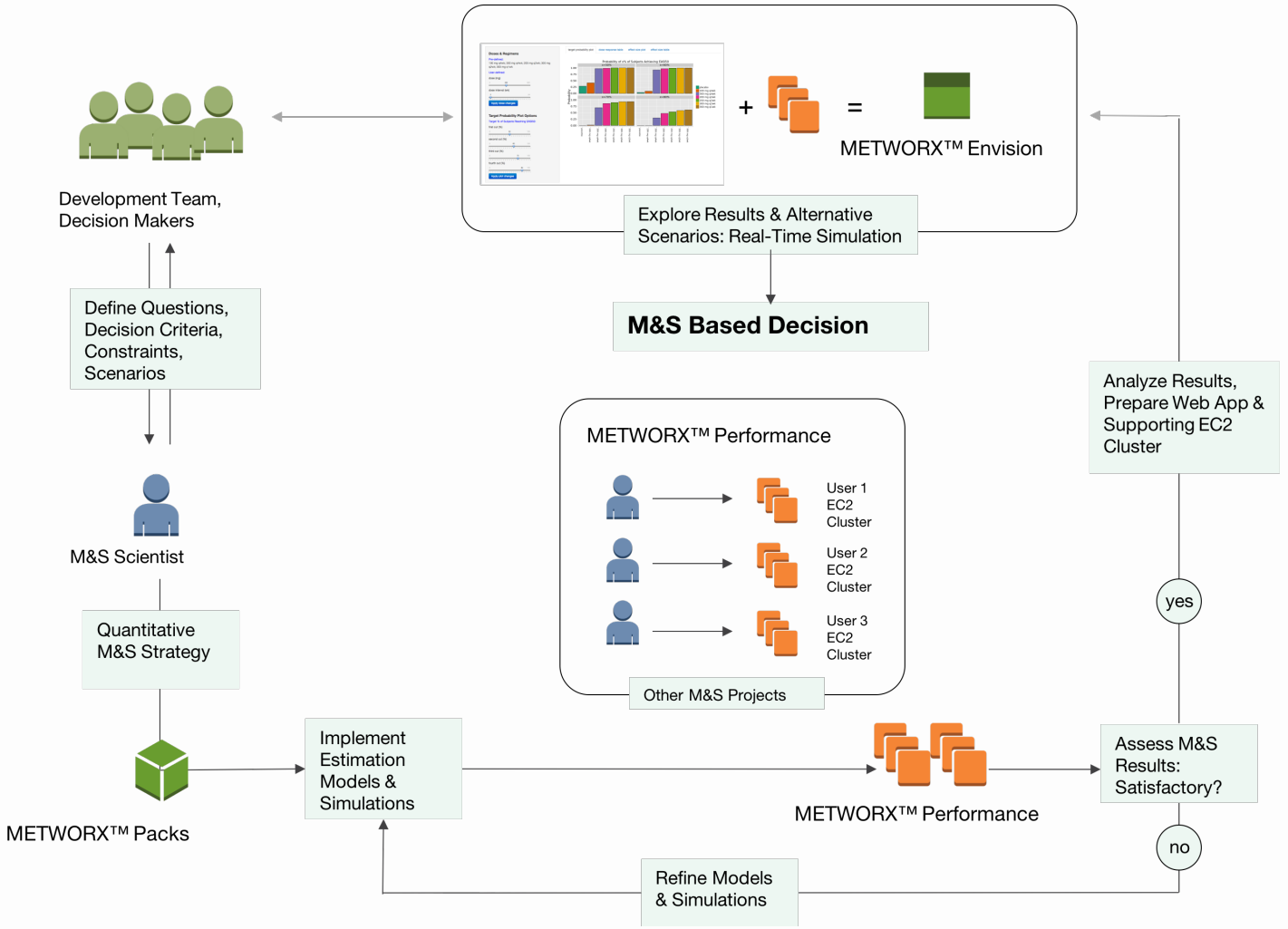


# Modeling and Simulation Based Decision Support:
# Typical Process Flow



# Harnessing the Power of Cloud Computing with Metworx Performance and Shiny Server Pro through Metworx Envision



# R Related Tools

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Shiny by RStudio

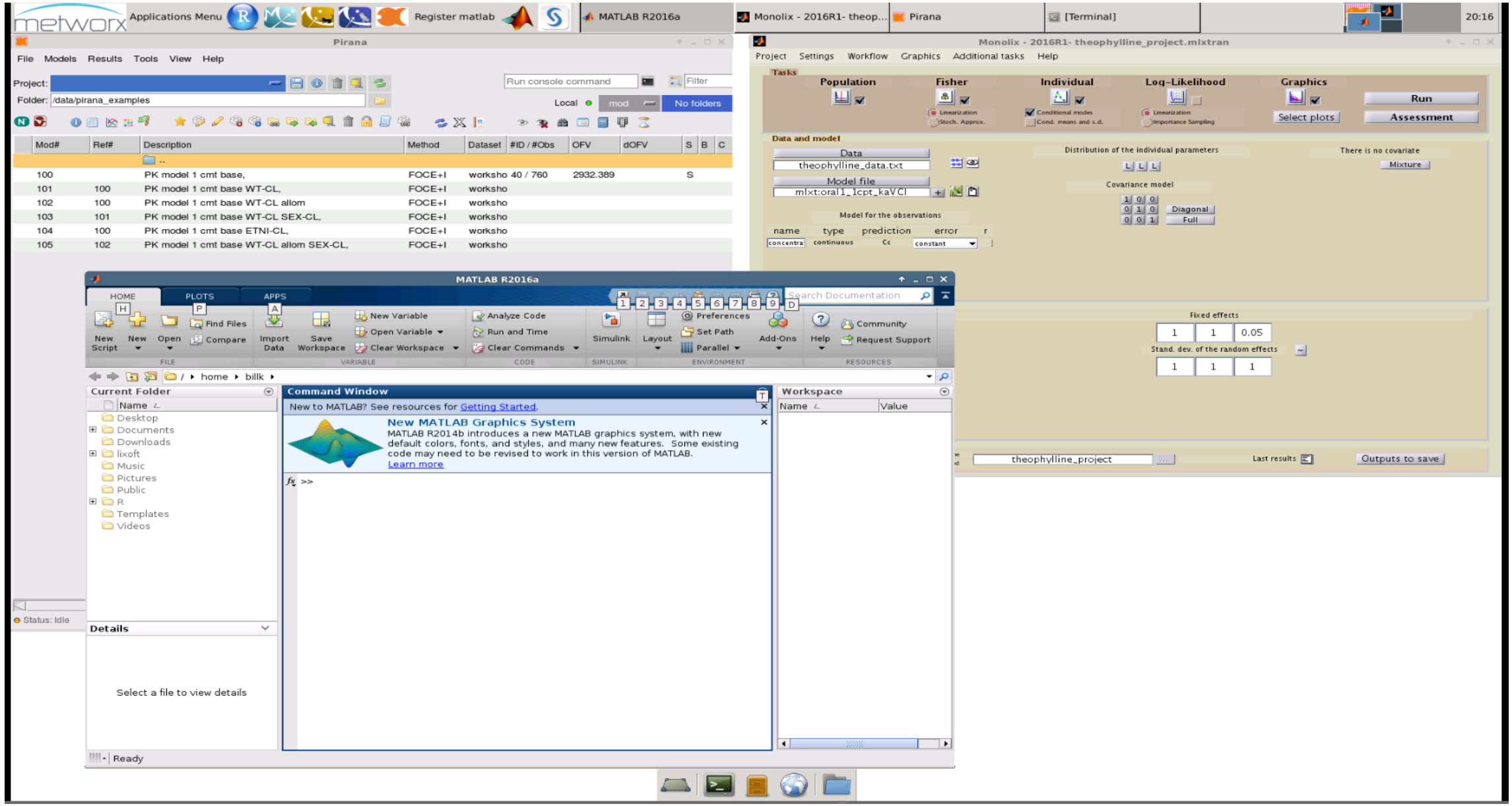
Web App (browser)

`qapply`

`mrgsolve`

`Rcpp`
`C++`
`ODEpack`

# Desktop Tools



# Vision for M&S Cloud-Based Platform

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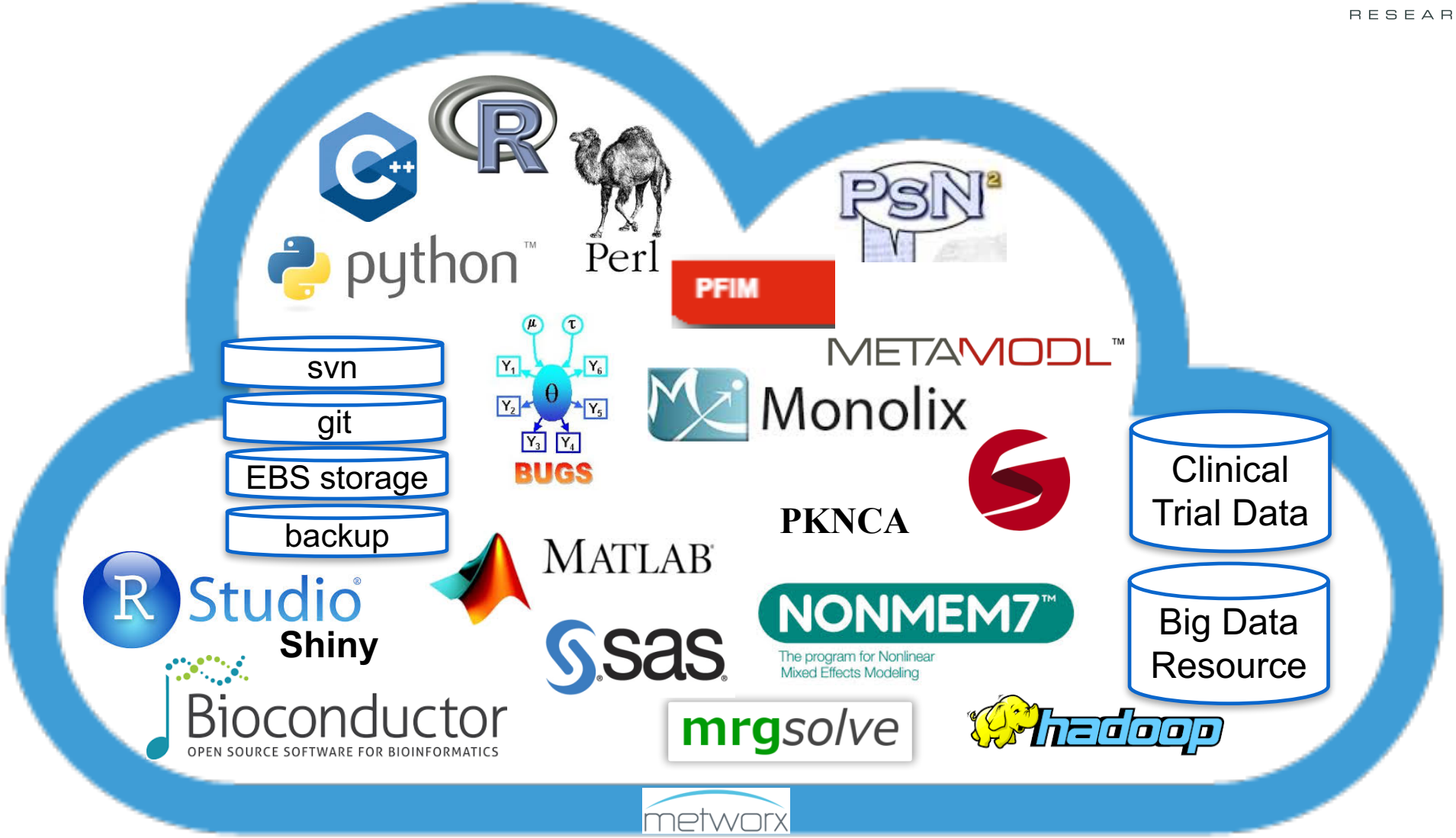


Computational Biology, Bioinformatics → Systems Pharmacology → PK-PD, Trial Simulation → Statistical Analysis → Comparative Effectiveness, Health Outcomes