CREDITS

UMC St Radboud

LEAD PHARMA

CMBI

University of Leicester

Vrije Universiteit Brussel

nbic

YASARA

CCPN

Spronk NMR Consultancy

sara

bitbrains IT SERVICES

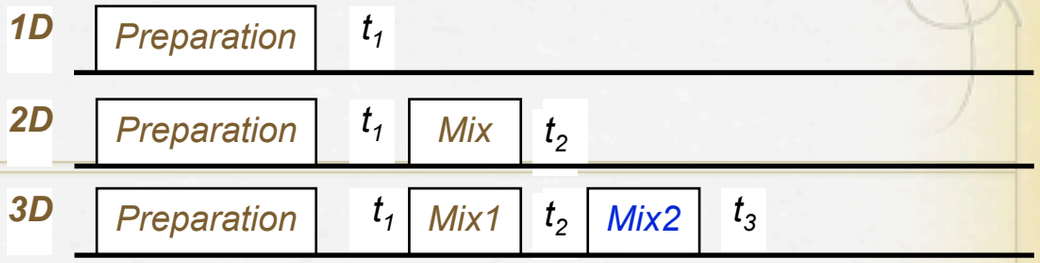
we-nmr

OVERVIEW

- Introduction
- Clouding
- Results
- Dreams

Molecular Biology

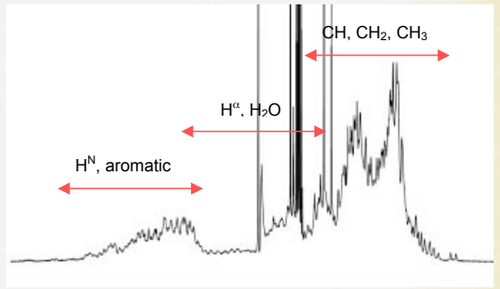
Spectroscopy

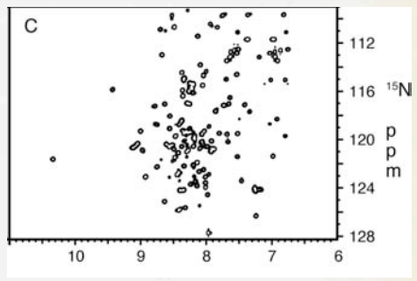


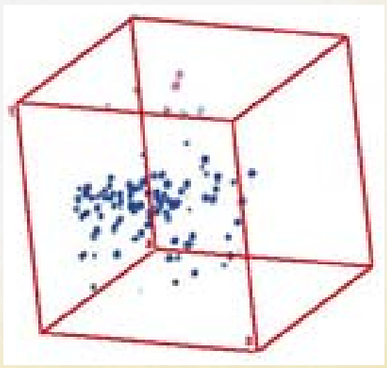
Biological question ?

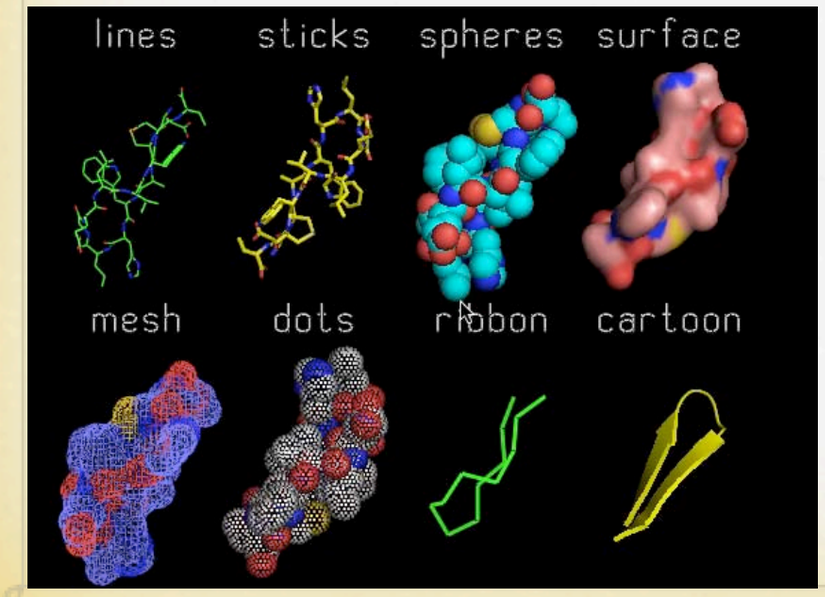
Structures
Interactions
Dynamics

Data



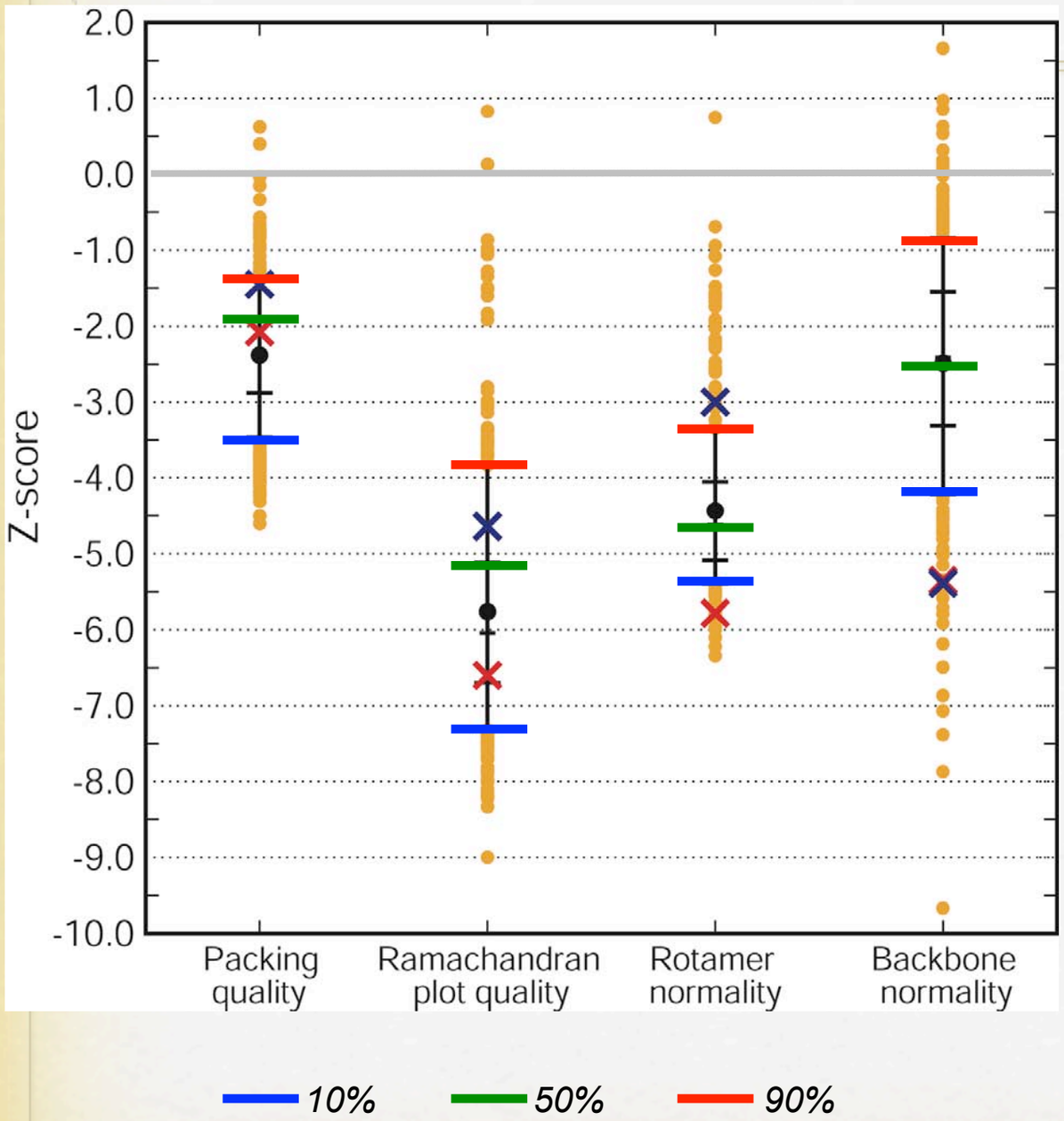






MOTIVATION

~600 Structural Genomics structures



- NMR structures are generally not very good. ~25 % of recently deposited structures is seriously flawed
- Structural quality can often be improved by:
  - Proper computational procedures
  - Validation of input data
  - Validation of results

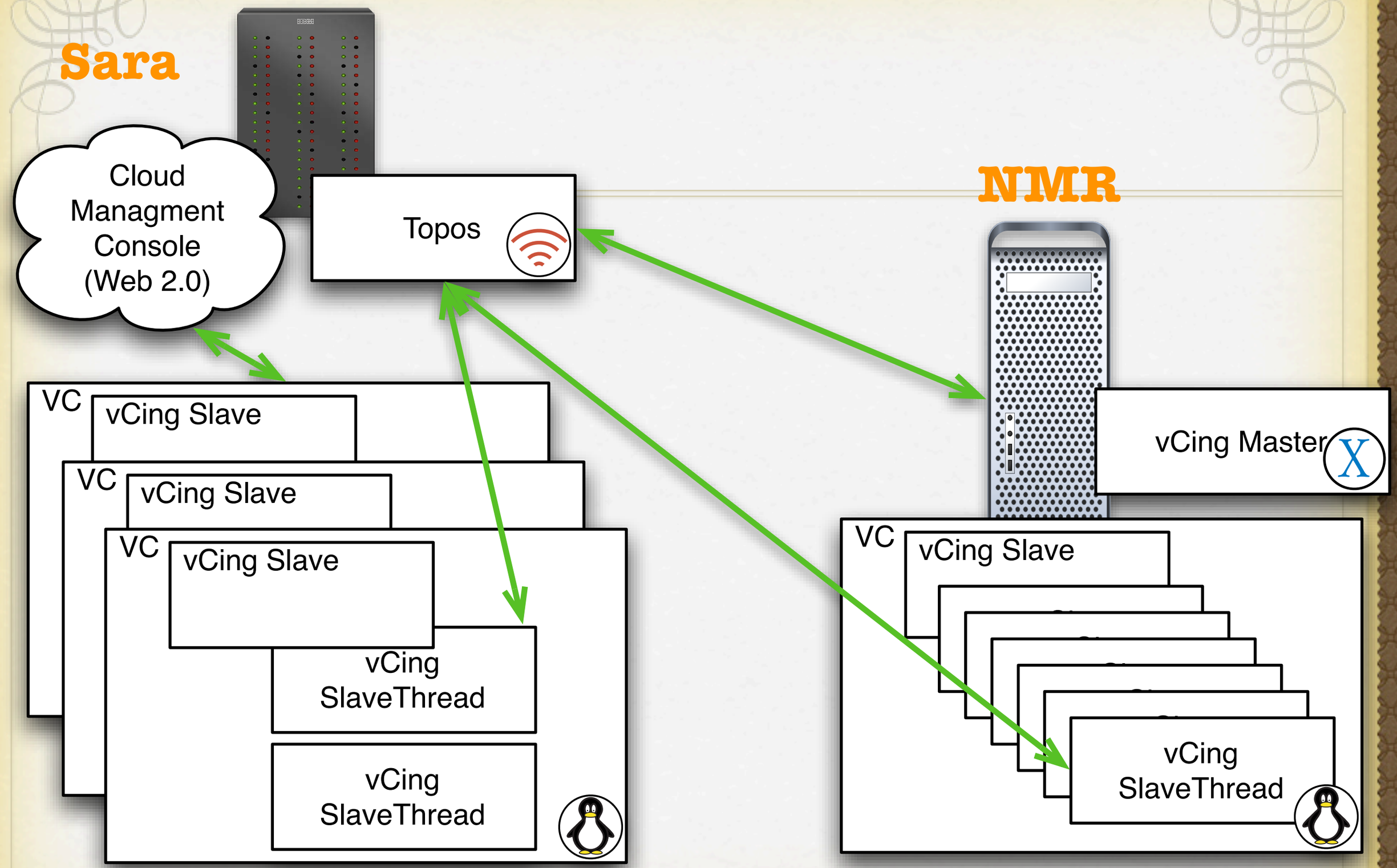
Nabuurs et al. PLoS Comp. Biol. 2, e9, 2006

WHY CLOUDING?

- Project needs ~25 programs so setup/updates Grid too tedious
- Disadvantages vanished
- Independence from hardware
- Easy addition of more slaves

CLOUD COMPUTING

- Sara & Bitbrains
  - Hardware and cloud management
- TOPOS (TOken POol Server)
  - Developed for grid computing
  - Backend server/database at Sara
- VC (Virtual CING) as the virtual machine


Sara
Cloud Managment Console (Web 2.0)
Topos
NMR
vCing Master
X
VC
vCing Slave
VC
vCing Slave
VC
vCing Slave
vCing SlaveThread
vCing SlaveThread
VC
vCing Slave
vCing SlaveThread

RESULTS

- First tests
  - Stress tested with 10k tokens on 17 VMs (34 nodes) finishing within 2 hours with test script.
- Production
  - Validation of 9k entries on ~25 VMs (50 nodes)
  - Average job was ~20 minutes and ~20 Mb
  - Total 16 core weeks done in 1 week

DREAMS

- NMR_REDO: improved database of NMR structures
  - Prior efforts done for 100 & 500 but now trying 5k+
- Tested with 90 entries in cloud setup
  - Average job was 10 hours and ~30 Mb
  - Quality indicators improved significantly
- Resources: Sara, Bitbrains, Condor and/or WeNMR

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