Emerging Campus Infrastructure at Virginia Tech

OSG All Hands Meeting 2012
Bill Marmagas
zorba@vbi.vt.edu

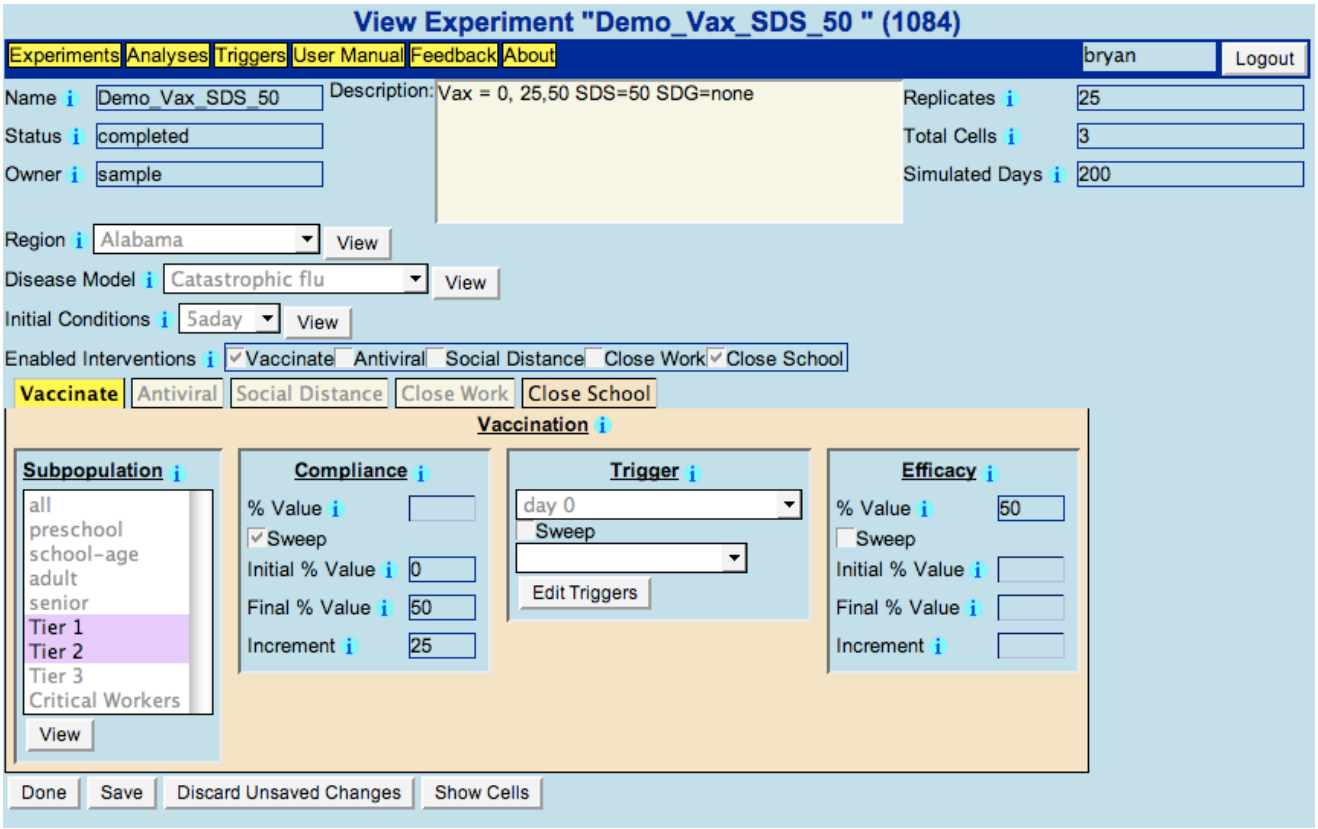
Advanced Computing and
Decision Informatics Laboratories

Virginia Bioinformatics Institute

- **ACDIL Division**
  - Modeling and simulation of *interaction-based*, *co-evolving* technical, biological, and social networks in support of national policy
    - Infrastructure, immunology and disease, public health epidemiology, and national security
  - Research Niches
    - Advancing the **math** & science of these simulations
    - Integrating **social and behavioral** modeling
    - Developing computational tools that leverage **HPC**

Example: DIDACTIC / EpiFast

- **Web-based epidemic modeling using HPC**



Major Funders

CDC
CENTERS FOR DISEASE CONTROL AND PREVENTION

NATIONAL INSTITUTES OF HEALTH

NSF

U.S. DEPARTMENT OF HOMELAND SECURITY

DEFENSE THREAT REDUCTION AGENCY
UNITED STATES OF AMERICA

Campus Infrastructure Pieces

- OSG Submit Host
- Campus Factory

OSG Submit Host

- **Flocks HTPC Jobs to OSG Via Engage**
  - RENCI Configured Host DN on engage-submit3
  - OSG Factory Also Configured to Allow Access
- **Host Certificate**
  - This Host Can Be A Shared, Multi-User Resource
- **Submit Host Firewall: Condor Config.**

  HIGHPORT = 65535

  LOWPORT = 44536

Submit File Example: EpiFast

```
universe = vanilla
executable = runepifast.sh

Requirements = (CAN_RUN_WHOLE_MACHINE =?= TRUE)
+RequiresWholeMachine = True

# Put a process run on Hold if it has been running for four hours:
periodic_hold =  JobStatus == 2 && (CurrentTime - EnteredCurrentStatus > 14400)

ShouldTransferFiles = YES
when_to_transfer_output = ON_EXIT
output = submit.htpc.Vac-0.05_Alloc.out.$(Cluster).$(Process)
error = submit.htpc.Vac-0.05_Alloc.err.$(Cluster).$(Process)
log = submit.htpc.Vac-0.05_Alloc.log.$(Cluster).$(Process)

#Process Run: 0
transfer_input_files = ../../../bin/EpiFast, ../../../bin/mpiexec, ../../../areas/
SeattleData.tgz, ../Vac-0.05_Alloc-0.0-0.0-0.0-0.0-1.0.tgz
arguments = 8 Vac-0.05_Alloc-0.0-0.0-0.0-0.0-1.0
queue
```

Campus Factory

- **Enables Flocking to Local HPC Clusters**
  - Jobs Glide In To Compute Nodes
- **Can Also Be An HTPC Resource**
  - echo "#PBS -l**nodes=1:ppn=8**"
    (/usr/libexec/condor/glite/bin/**pbs_local_submit_attributes.sh**)
  - Moab NODEACCESSPOLICY=SINGLEJOB does same
- **Same EpiFast Jobs Run Here**

Latest Campus Factory 0.4.3

- **Prevents "Walltime Rogues"**

  SHUTDOWN_GRACEFUL_TIMEOUT = 72000

  MAXJOBRETIREMENTTIME = 34800

  - 72000 sec. + 34800 sec. = 29 hours 40 minutes

  ./glideinExec/glidein_startup -dyn -f -r 1200

  - 1200 min. = 20 hours run time for condor_master

  echo "#PBS -l**walltime=30:00:00**"

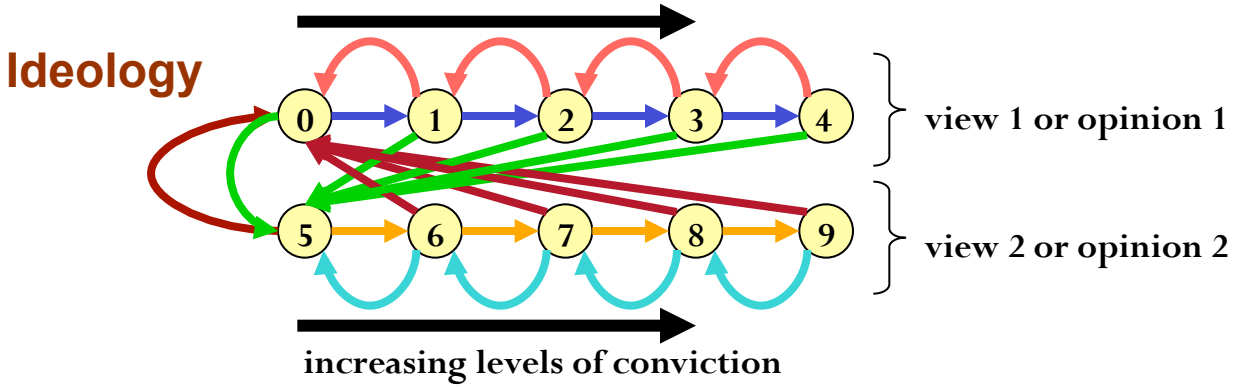
  - 30 Hour Walltime is a bit more than SHUTDOWN_GRACEFUL_TIMEOUT + MAXJOBRETIREMENTTIME

Future Work

- **Infrastructure**
  - Add Second Campus Factory Cluster
  - Integrate Campus Factories Into Submit Host
- **Web Interface Plug-In to Submit Host**
- **More Applications**
  - Computational Social Science Example
  - Biochemical Network Simulation Example

Discrete Dynamical Systems

- **Application: Model group dynamics and how a population may or may not reach a majority view.**



- **75879-node Epinions Network = 10^{75879} Config's**
  - We can look at a smaller, statistically significant set
  - Perhaps: 100 Config's X 50 Simulation Time Steps
- **Clusters of Muticore (Worker and Slave) Jobs**

COPASI

- **A software application for simulation and analysis of biochemical networks and their dynamics.**
  - A collaboration between VBI, the University of Heidelberg, and the University of Manchester

- **Condor-COPASI is a web-based interface for integrating COPASI with Condor**
  - Potential good fit to flock to a dedicated Campus Factory to submit to their cluster queue

References

TWiki: CampusGrids/InstallCondorFlockSubmit

TWiki: Documentation/CampusFactoryInstall

Bill Marmagas
Senior Systems Engineer
Network Dynamics and Simulation Science Laboratory
Virginia Bioinformatics Institute
zorba@vbi.vt.edu