



*Richard D. Berlin*  
**Center for Cell Analysis and Modeling**

*National Technology Center for Networks and Pathways*

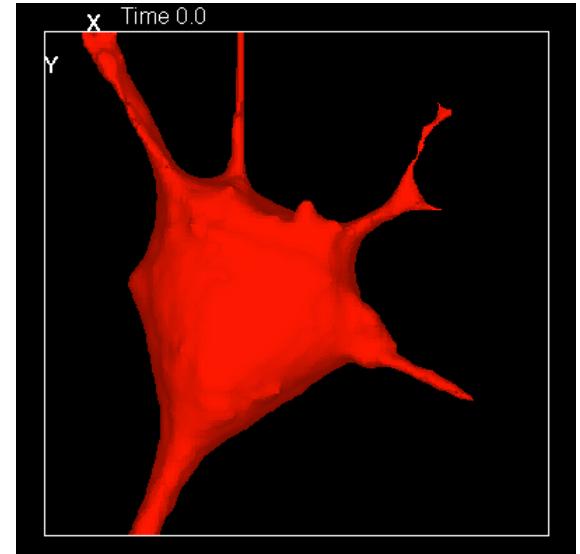
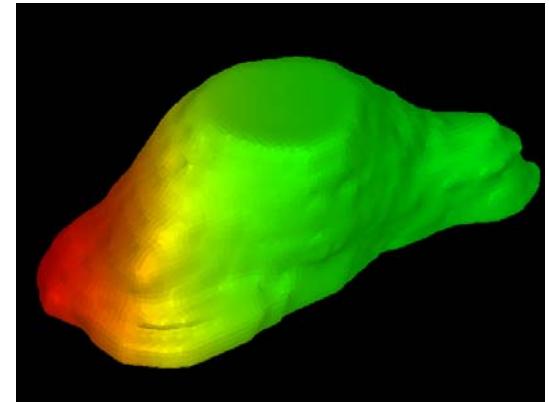
# CompBioGrid VO

Jim Schaff

Lead Developer – Virtual Cell Project  
University of Connecticut Health Center

# CompBioGrid VO

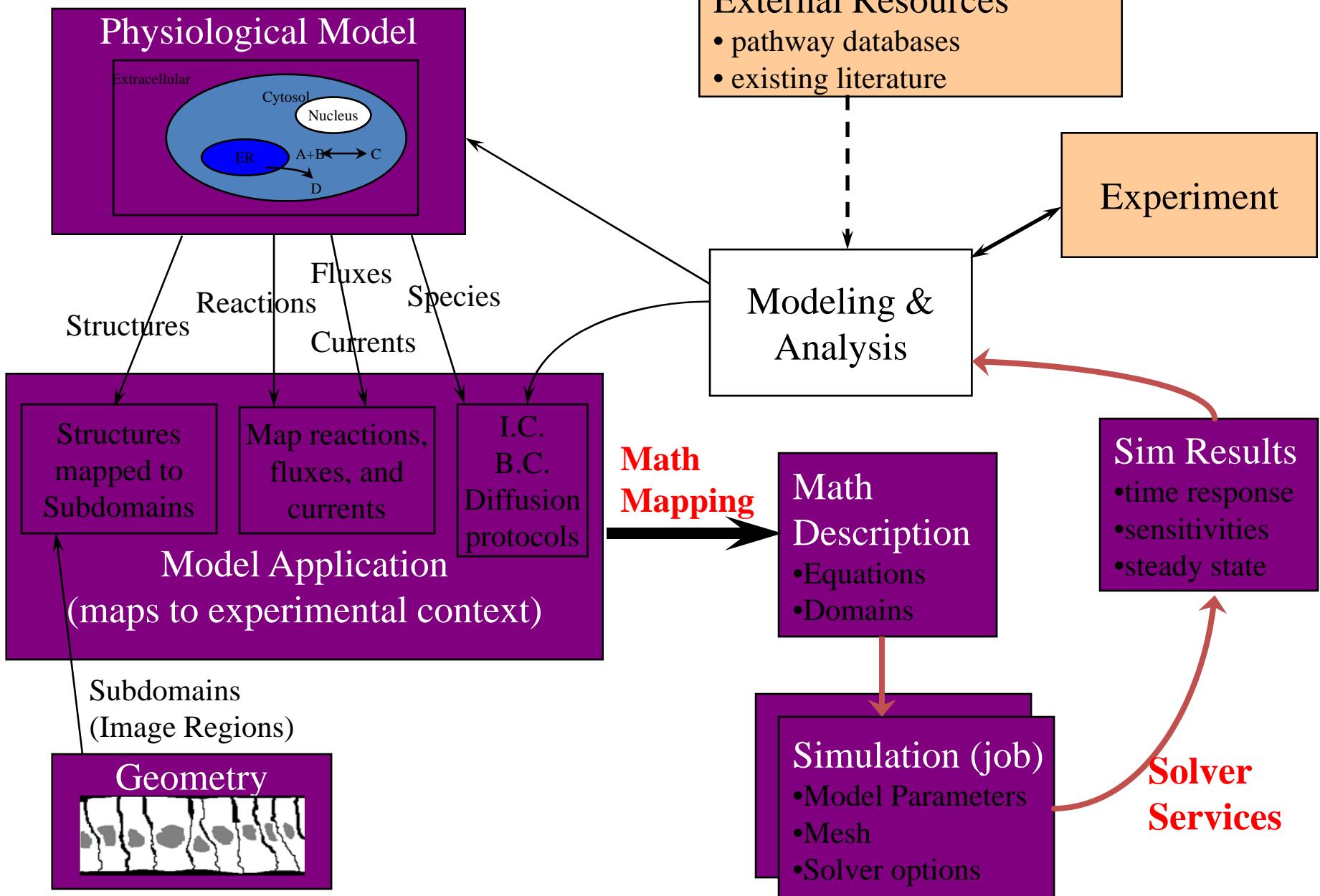
- Virtual Organization
  - <http://CompBioGrid.org>
  - VO manager (**Ion Moraru**)
  - VO operations contact (**Fei Gao**)
  - SysAdmin (**Jeff Dutton**)
  - VCell Application (**Jim Schaff**)
- Scope (VCell and beyond):
  - Molecular Complexes ← Cells → Tissues
  - Biochemistry, Diffusion, Advection, Electrophysiology, Cytoskeletal Dynamics, Cell Motility
  - Stochastic/Deterministic
- Motivation - Computationally Expensive
  - Arbitrary 3D Geometry
  - Multiple spatial scales
  - Multiple time scales
  - Multiple Trials (Stochastic)
  - Parameter Studies (Deterministic)

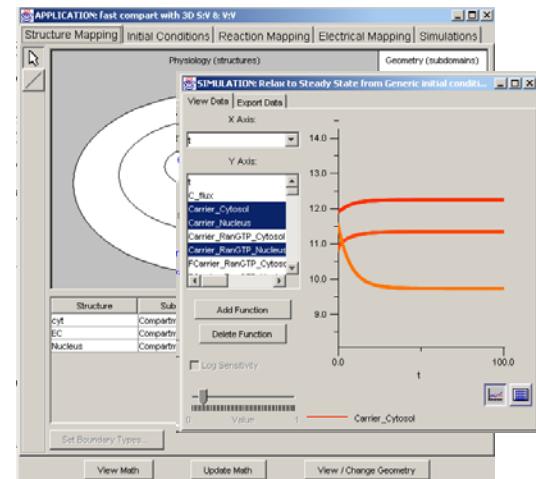
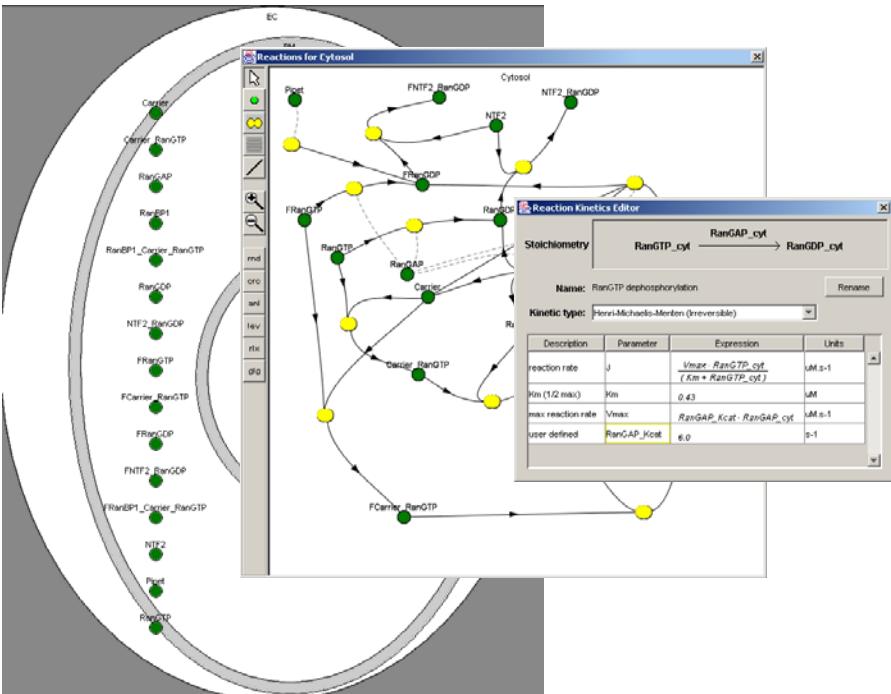


# Scope of VCell Project

- Intended Users
  - Biologists
  - Biophysicists/Mathematicians
- Modeling Domain
  - Compartmental or 1D, 2D, 3D Geometry
  - Reaction/Diffusion/Advection/Membrane Transport
  - Electric Potential (electrophysiology)
  - Membrane Diffusion
  - Parameter Estimation (1 month)
  - Stochastic (6 months)
  - Rule based modeling (via BioNetGen)
  - Adaptive Mesh Refinement (Chombo) (1 year)
  - Cell motility (>1year)
  - Generalized Multiphysics Framework (>1 year)

# Modeling Process

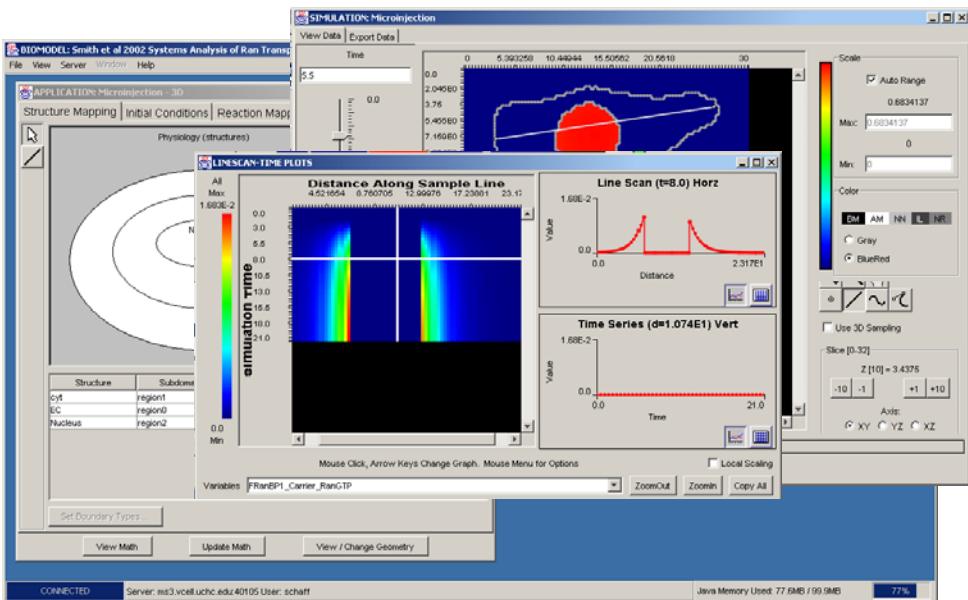


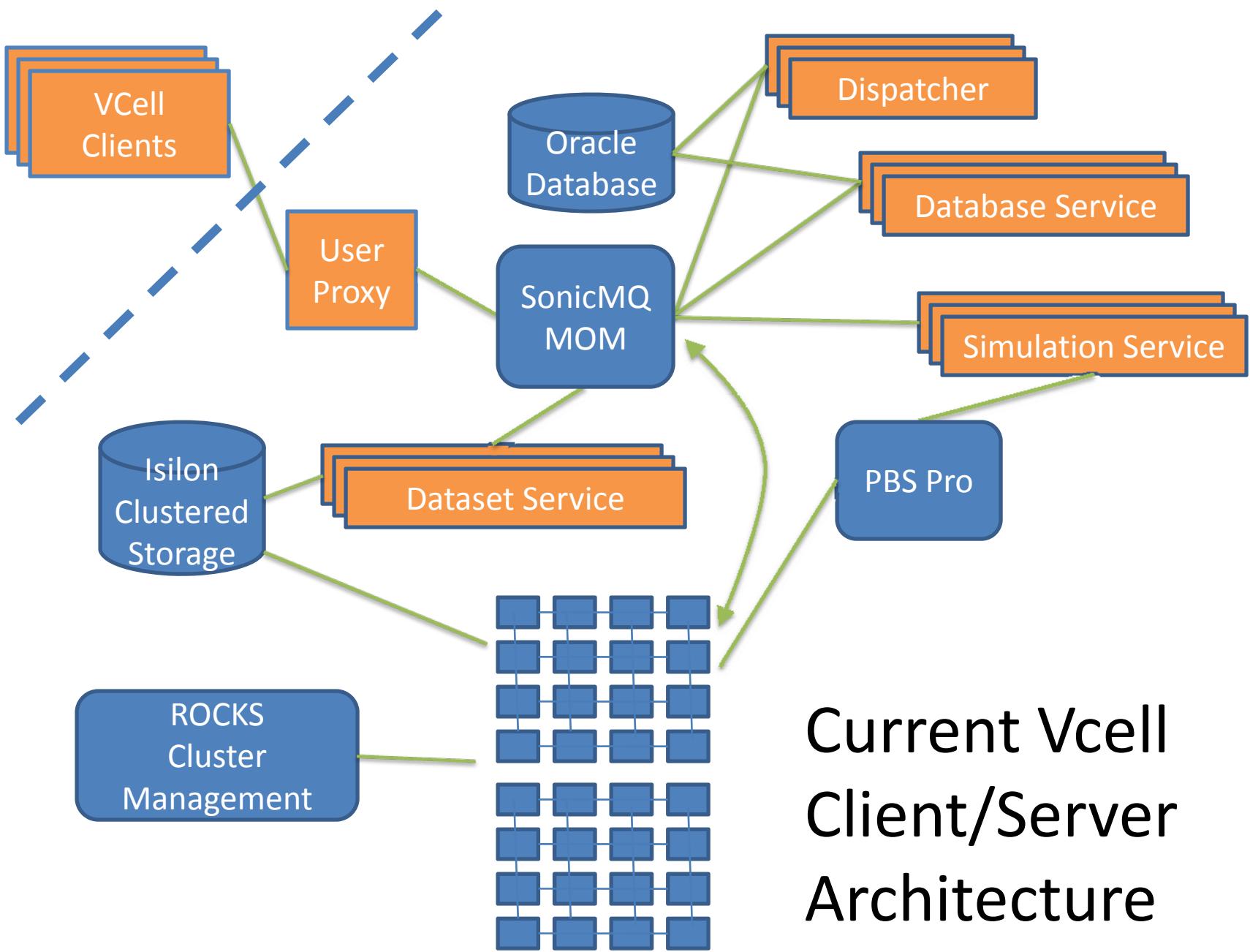


single model  
locations/molecules/mechanisms

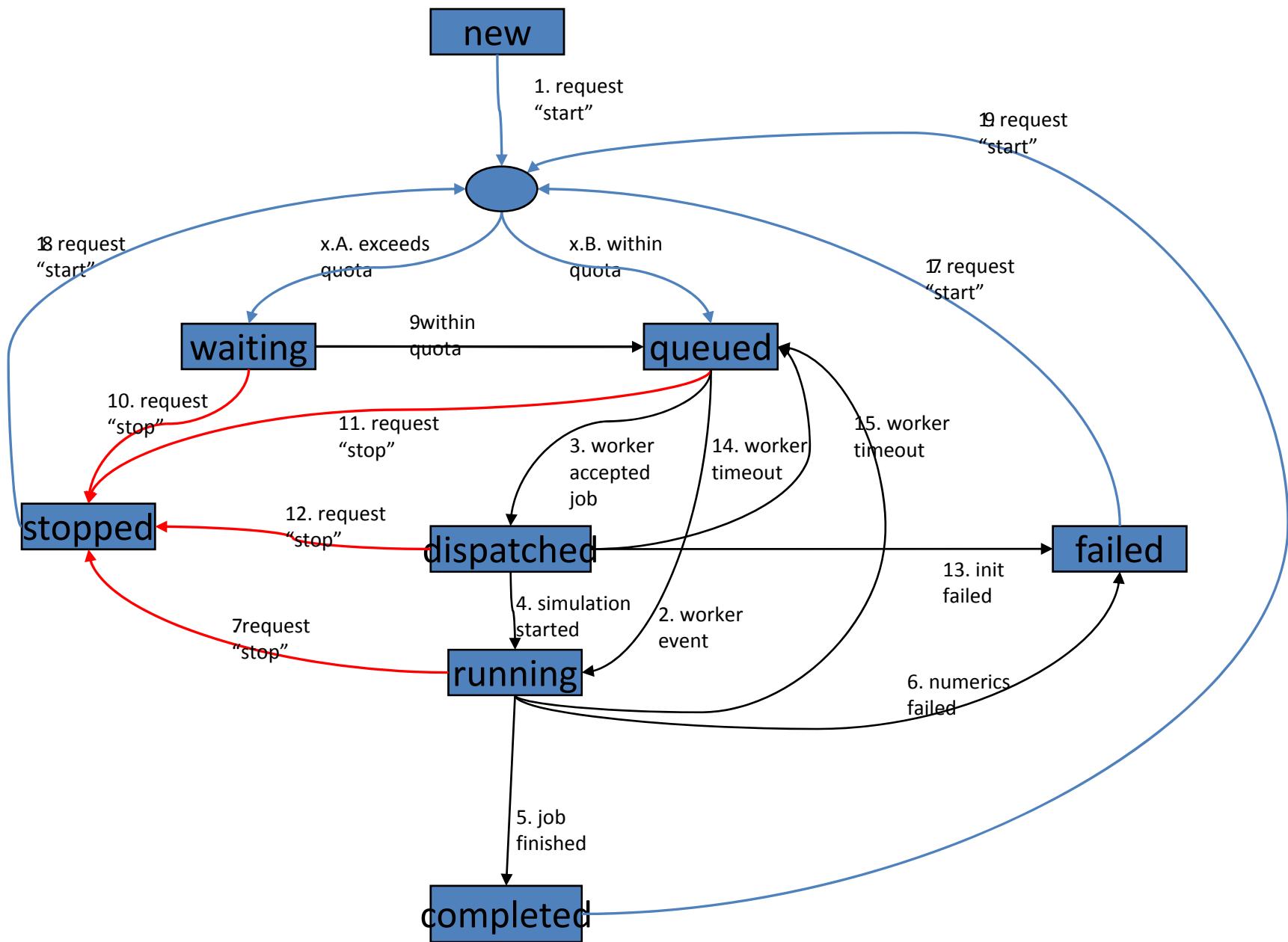
non-spatial apps  
ODEs, sensitivity analysis  
multiple simulations

spatial apps  
1D,2D,3D PDEs  
reaction/diffusion/advection  
multiple simulations





Current  
Vcell  
Client/Server  
Architecture



# Virtual Cell Job Scheduling

- **Multi-User Performance of current architecture**

- **Reliability**

- Job Monitoring, automatic restarting (3 times)
    - User Resubmission.
    - Task definition and status stored in database.
    - Persistent/Transactional message queues.

- **“Real Time” feedback to users**

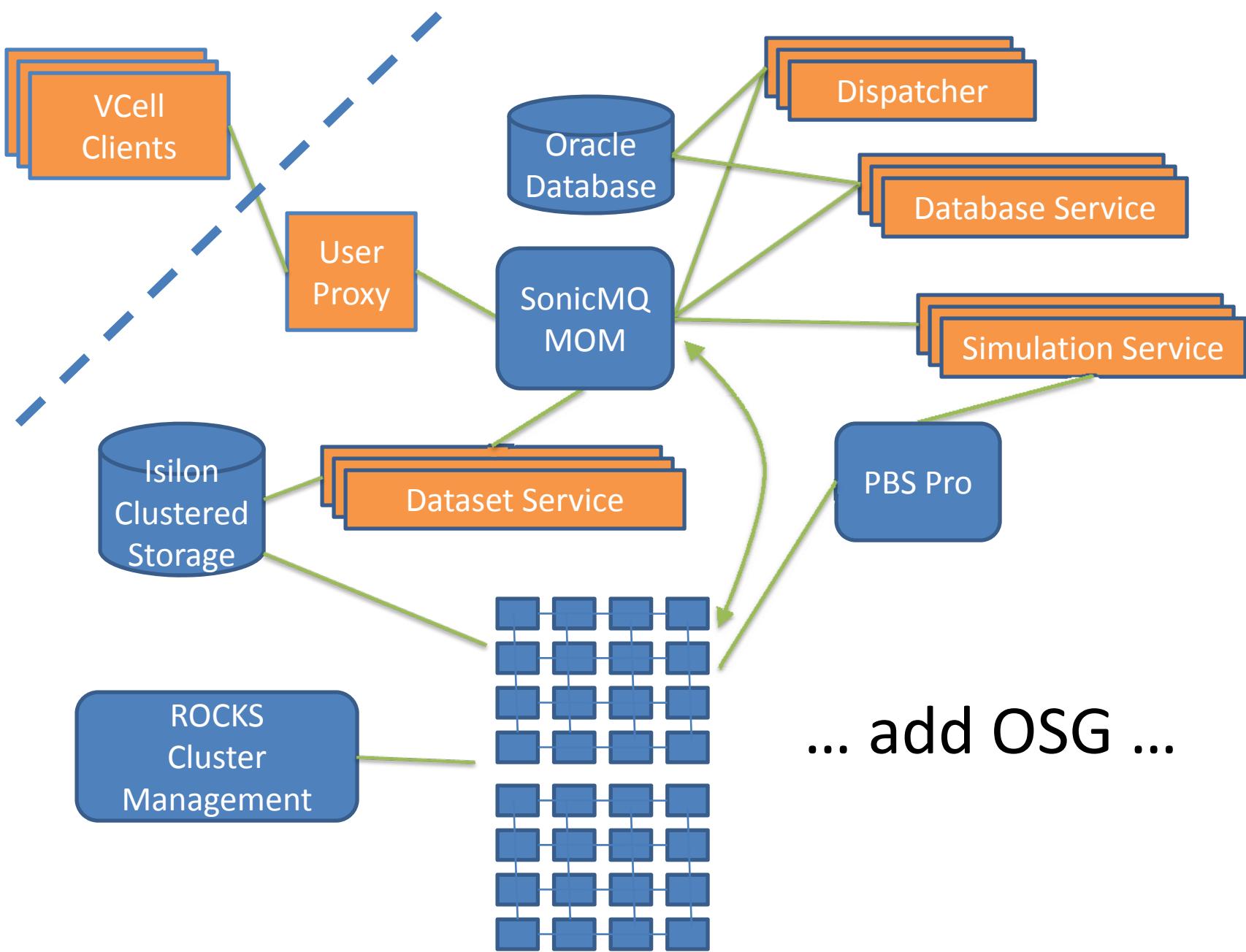
- Job Status (Progress Bar, Messages)
    - partial simulation results (stop/restart)
    - Simulation Checkpointing.

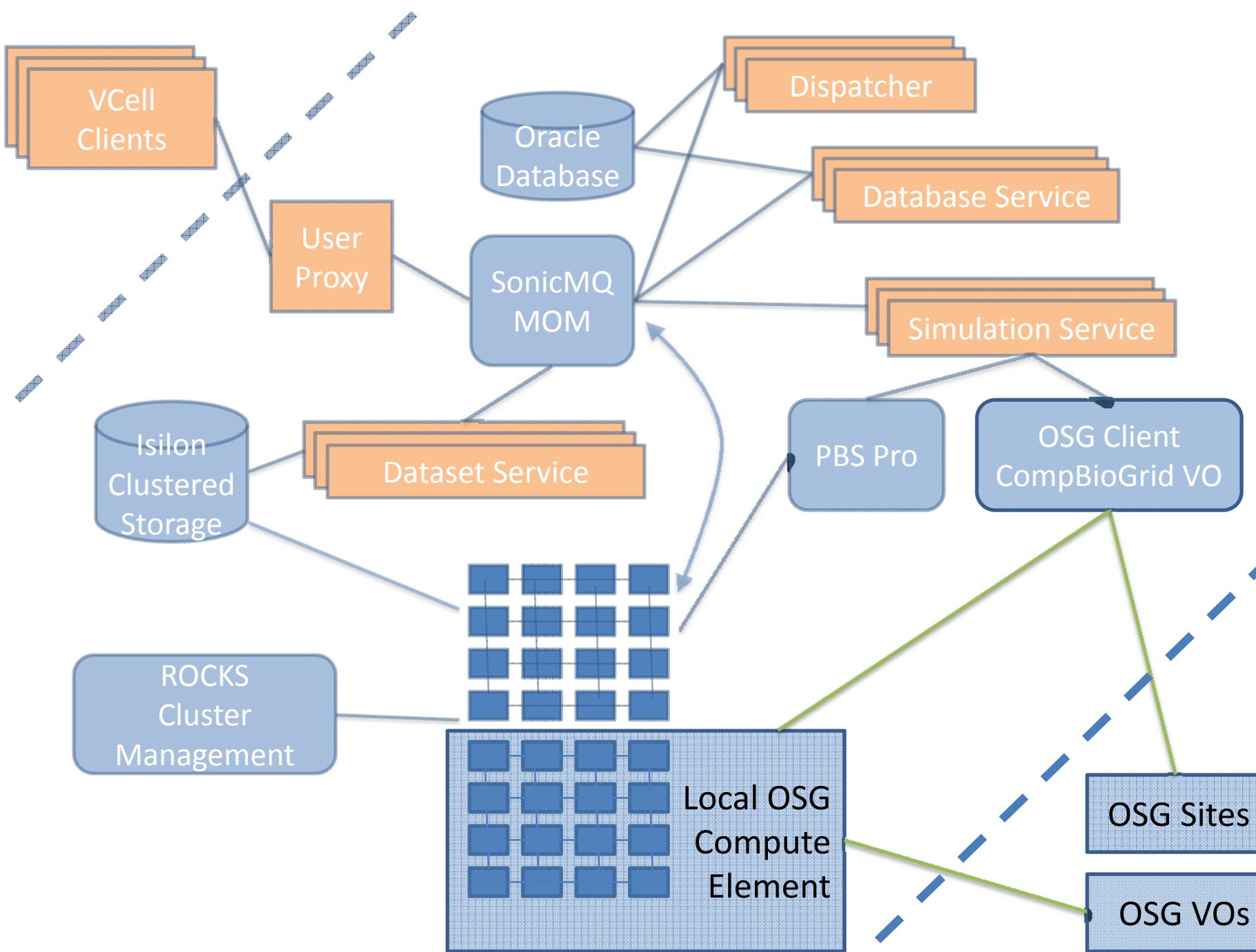
- **Scalability**

- Immutable objects promote caching
    - Stateless services – pull model for load balancing.
    - Services scheduled via PBS.

- **Policies**

- Database mediated Authentication/Authorization
    - Fixed User Job Quotas
    - Avoids “denial of service” by few users.
    - **too conservative ... idle machines.**





# Computational Resources



Younger Ion - Older Hardware

## Current Configuration:

Rocks Cluster > 300 Cores  
Clustered Storage > 50TB  
32 & 64 node SMPs  
2 x 40KW UPS/PDUs  
25 Tons cooling ++  
Enterprise Switching  
Dedicated Gb link to Internet2

## CompBioGrid VO

(to integrate with production  
Virtual Cell)

## UCHC CE

(trial installation of VDT)

# Acknowledgments

- OSG Initiative
  - <http://CompBioGrid.org>
  - Ion Moraru (VO Manager)
  - Jeff Dutton (SysAdmin)
  - Fei Gao (VO Operations Contact)
- VCell Team: <http://vcell.org>
- NIH (NCRR)

