

# VO Feedback

## The UCSDGrid “VO”

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# What is the UCSDGrid “VO”

In a nutshell

**A bunch of non-CMS UCSD users  
who use a glideinWMS instance  
to run on OSG**

# Some background

- The HEP department @UCSD is a strong believer in OSG
  - We have Frank W. on the Executive team
  - We run the CMS Analysis Frontend
  - We run the OSG glidein factory
- So we decided to spread the word around the UCSD campus and see if anyone was interested in using the OSG

# We found interest

- Talked to many people
- And found a very interested group
  - The Center for Theoretical Biological Physics  
<https://ctbp.ucsd.edu/>
  - With a strong champion  
Robert Konecny

# What we did?

- CTBP provided a submit node
- Engage created a group in their VOMS for us
  - The UCSDGrid “VO” is really the UCSDGrid group in Engage
- We got a pilot proxy
  - And registered it with the Engage VOMS
- Installed a Frontend on the “submit node”
  - Everything, including the CM and frontend

# Where do we run

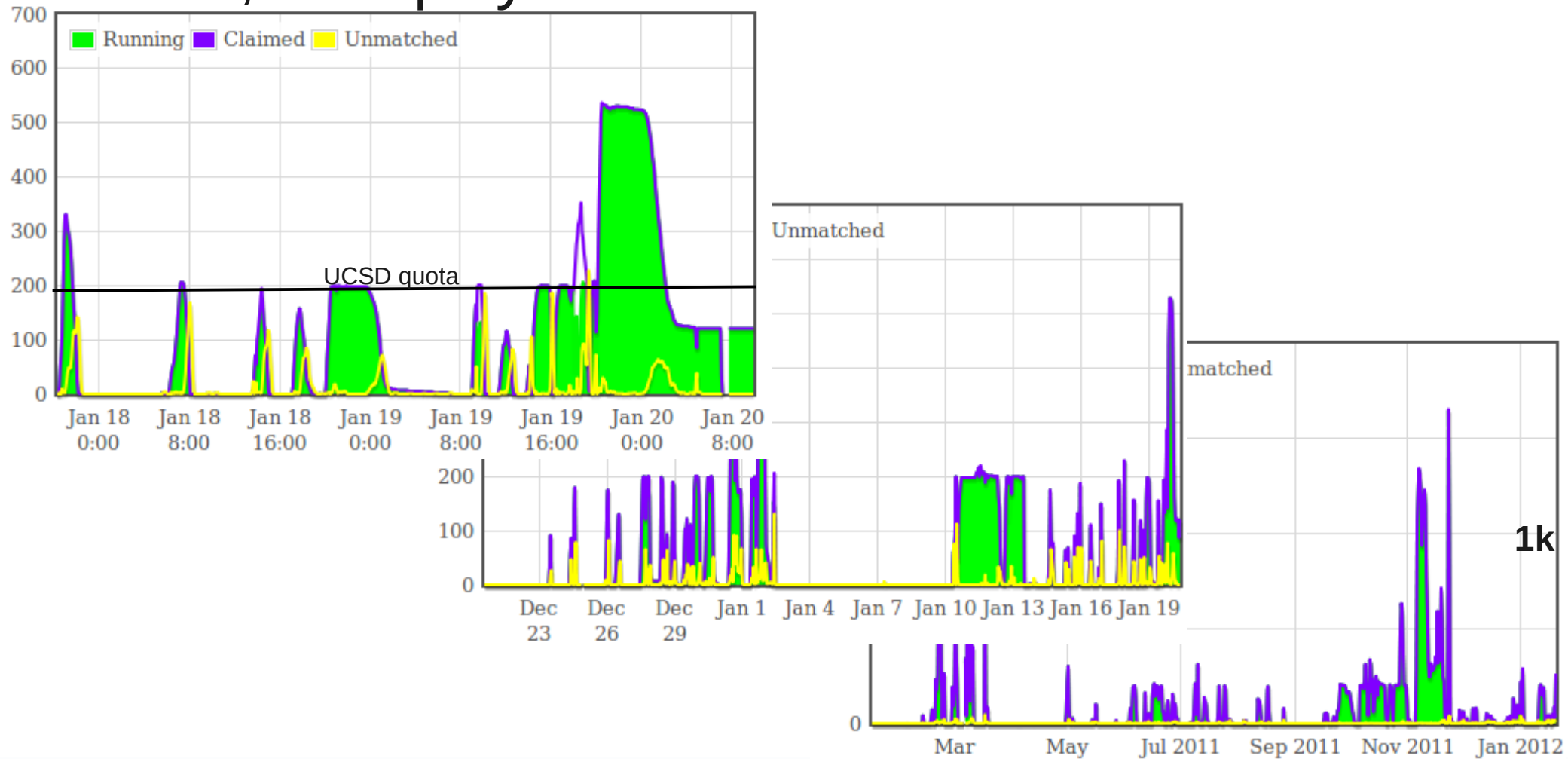
- Mostly UCSD CMS T2
  - Easier for data handling
- But users have the option to run on non-UCSD OSG sites
  - They just need to advertise  
`+DESIRED_Sites=any`

# How do users submit

- Ssh login into the submit node
  - condor\_submit
- Nothing fancy
- We have not “Gridified” our users
  - No user proxies!
  - **So we cannot use glexec**

# Is it used?

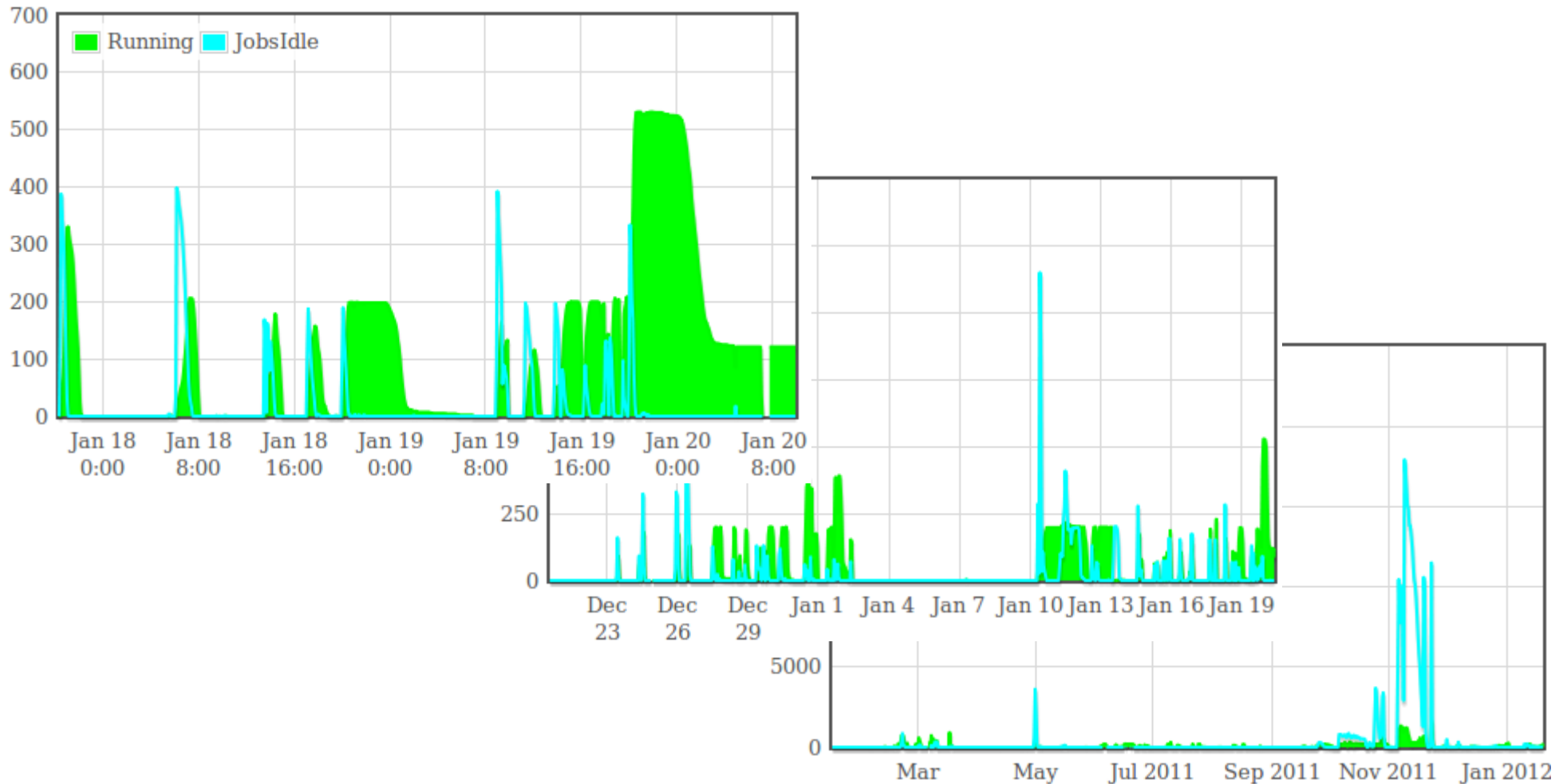
- Yes, but spiky!





# Use history

- Most jobs start within minutes



# Who are our users?

- The main users are the CTBP users, with most active being
  - Ryan Hoffman
  - Nick Schafer
- But we have a bunch of other users from various departments @UCSD
  - The CTBP gracefully agreed to allow us to use their submit node for all of them

# Ryan Hoffman

Our group develops simplified (but accurate) energy functions for the molecular dynamics of proteins. Instead of explicitly representing all protein and solvent atoms, our coarse-grained models treat only a subset of protein atoms using implicit solvation. Protein-protein interactions can change markedly depending on whether they are occurring in a solvated or desolvated environment; this basic fact is explicitly accounted-for in our models. We have recently added a major refinement to our solvation model: the incorporation of desolvation barrier. This desolvation barrier allows us to model the pressure-dependence of protein folding. OSG has expedited the sampling of our energy function for many external pressures and a handful of model proteins, in turn allowing for novel comparisons between experimental observations and our theoretical-computational predictions.

# Nick Schafer

I am using the OSG to study protein folding. In particular, I use many serial simulations to explore the global energy landscape and make direct measurements of kinetics on the spectrin repeat proteins, which are proteins that have been shown in experiment to be unique in that they have very similar structures and stabilities but vastly different kinetics.

# Fruitful collaboration

- UCSD local users very happy with the interaction with OSG
  - Get a lot more done than what they were used to
  - Especially the CTBP users
- CTBP decided to move all new purchases in the HEP OSG Cluster  
(Adding 72 cores right now)
  - So they don't need to maintain them
  - Not requesting special config or priorities

# Frontend config

- Pretty basic
- Just two groups
  - UCSD
  - Offline
- Looking for the `DESIRED_Sites` attribute in the job classad

# Praise and problems

- **It just works**
  - Hardly even need to check on it
  - Like once a month at most
  - But I do send myself a daily email
    - to make sure jobs are starting
    - Since we are spiky
- No major complains

```
condor_q -format '%s ' Owner
          -format '%i ' JobStatus
          -format '%i\n' NumJobStarts
| sort |uniq -c
| mail -s "$DATE" $EMAIL
```

```
66 cfeng 1 0
38 cfeng 2 0
75 cfeng 2 1
```

**THE END**