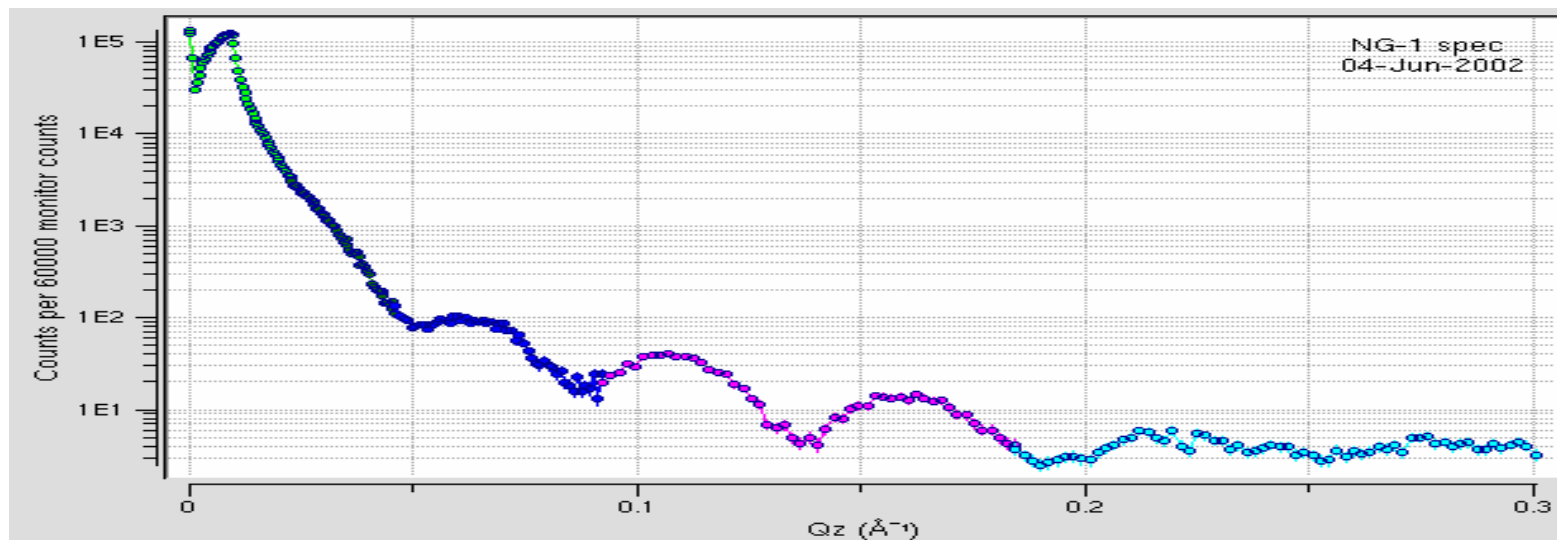
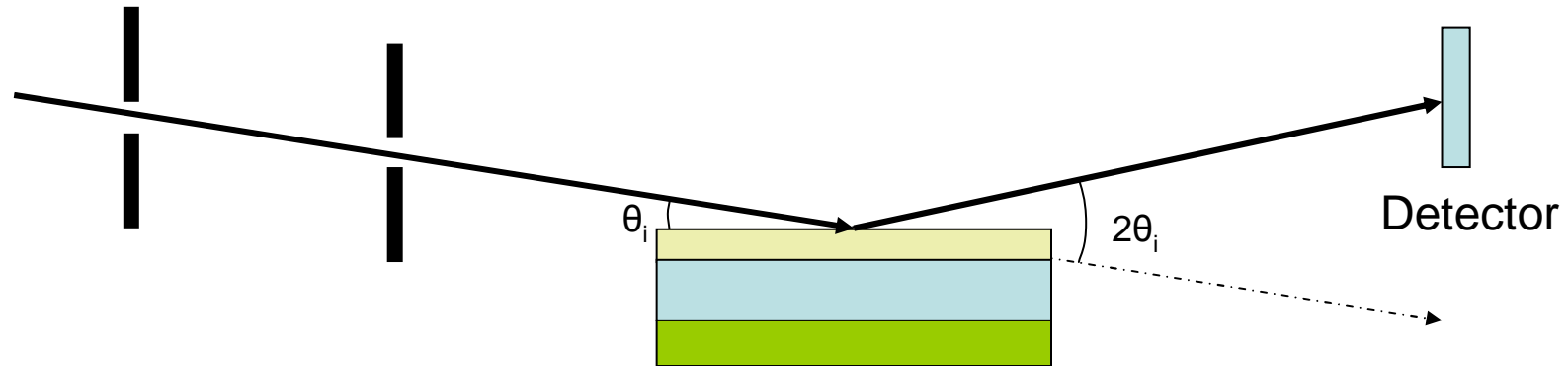


# Danse Reflectometry

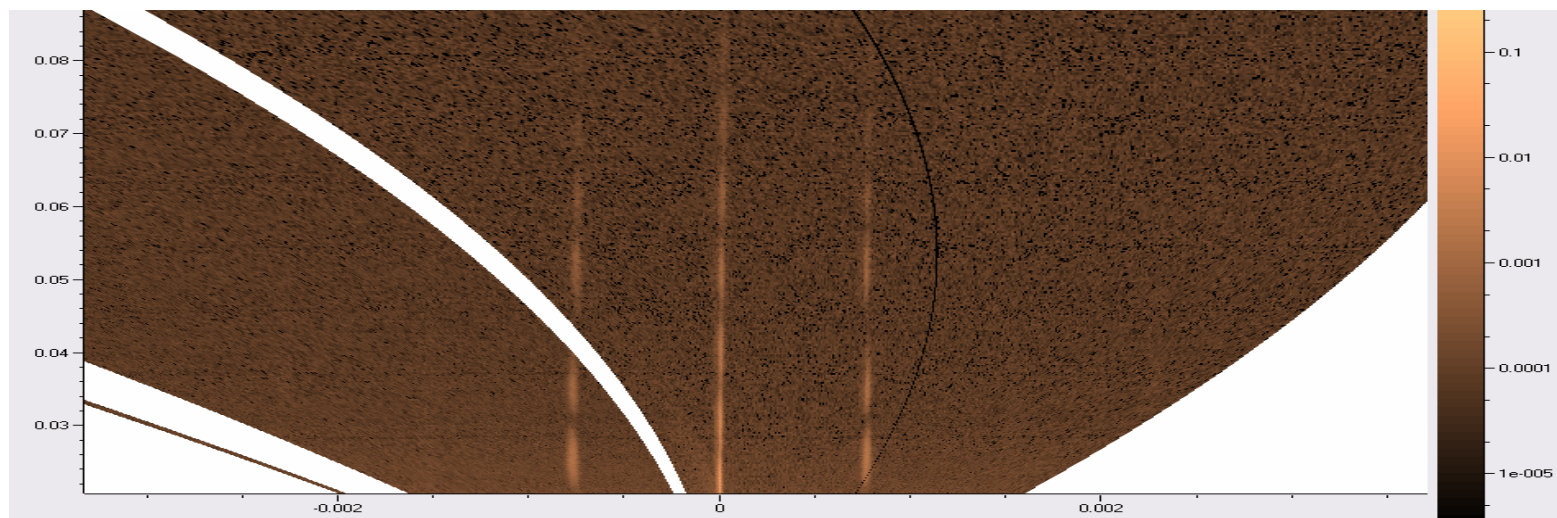
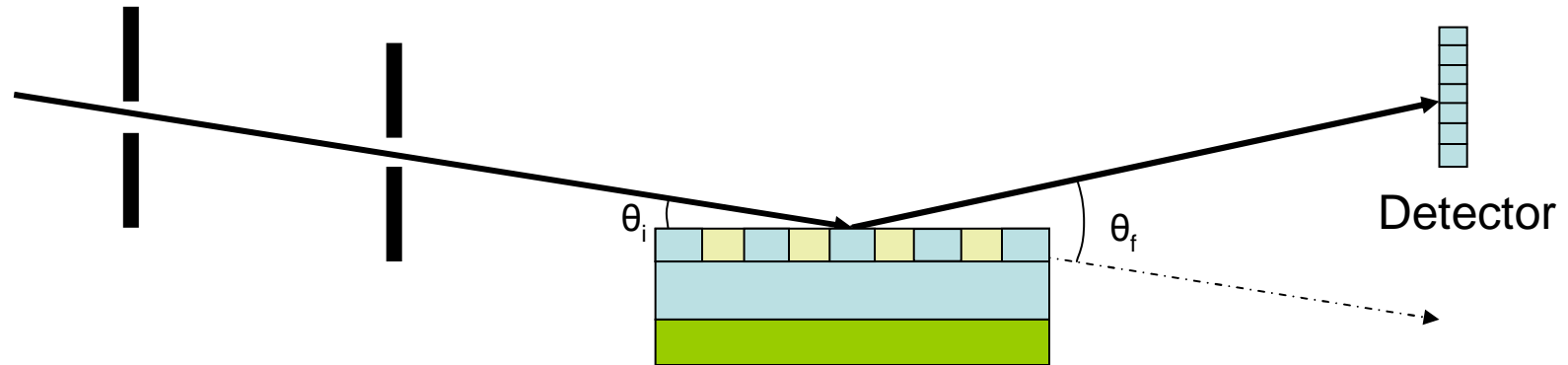
Paul KIENZLE, Wenwu CHEN, Ziwen FU  
Christopher METTING, David TIGHE  
Reflectometry Computing Group  
University of Maryland/NIST



# Reflection from Layers

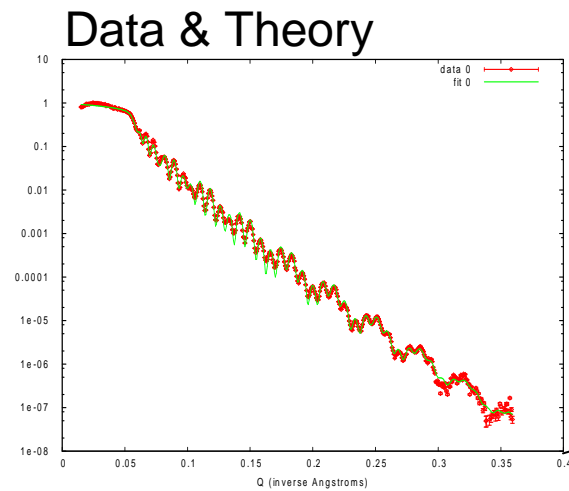
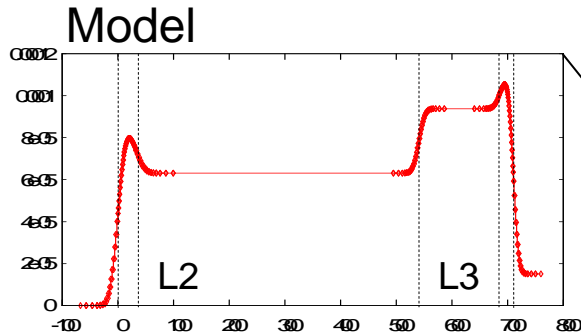


# Reflection from Grating

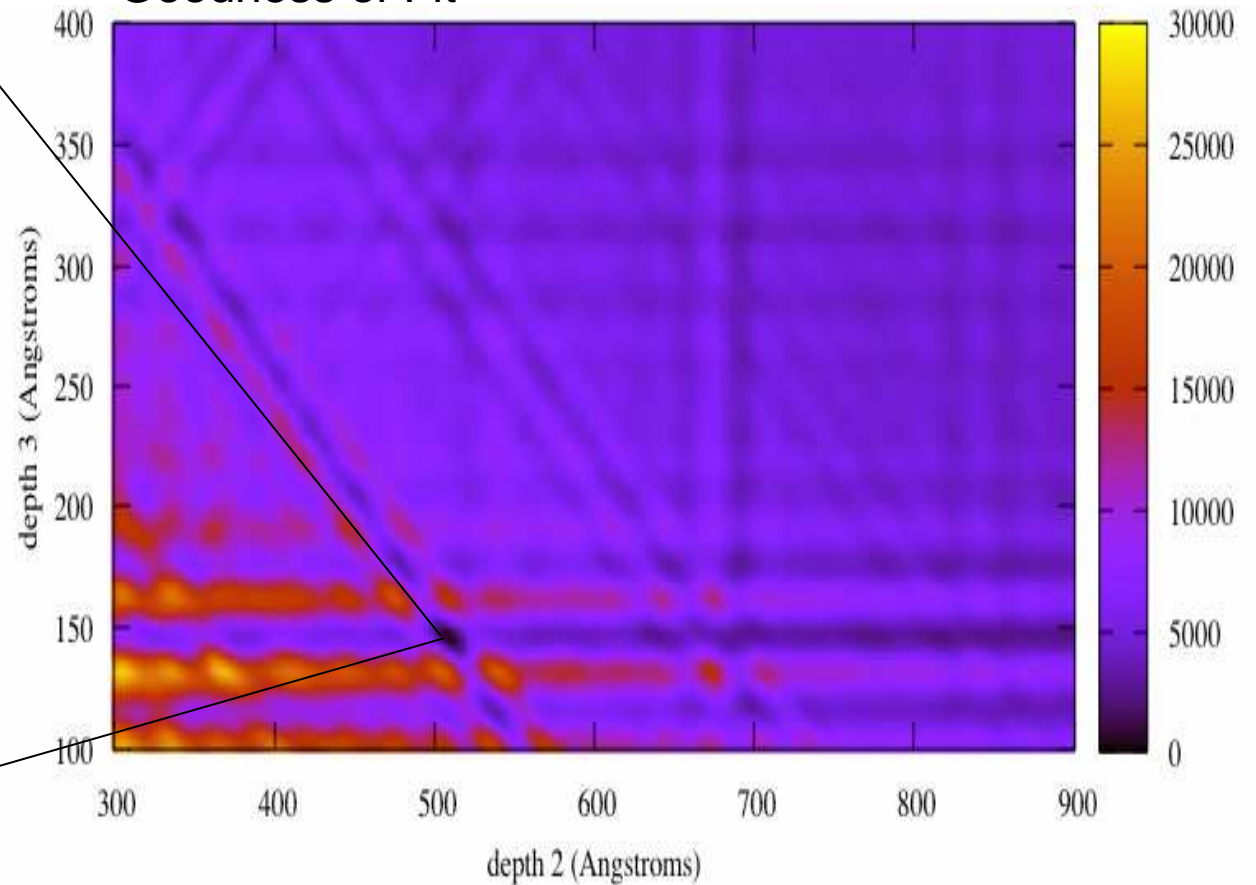


Offspecular Reflectivity

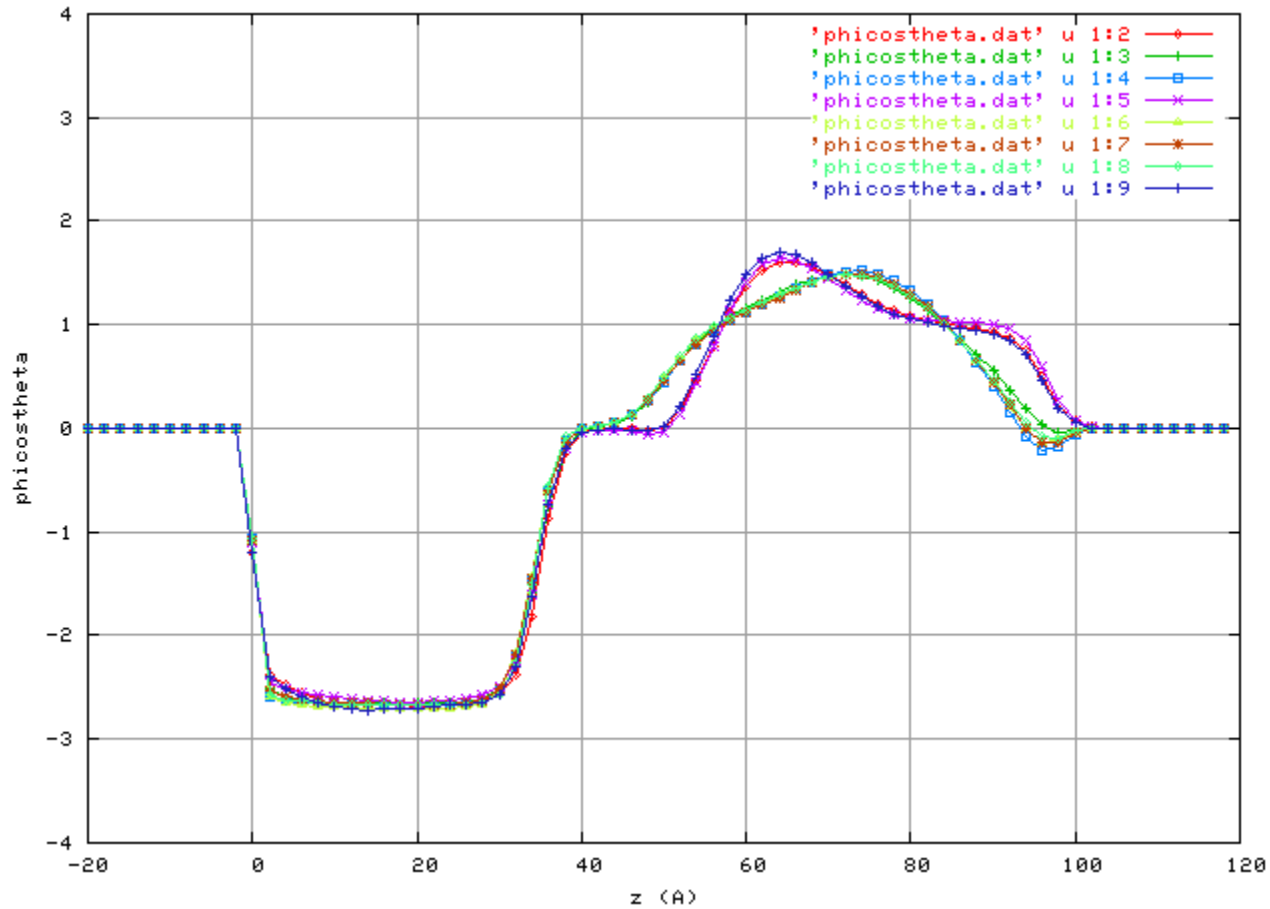
# Global Fitting



### Goodness of Fit



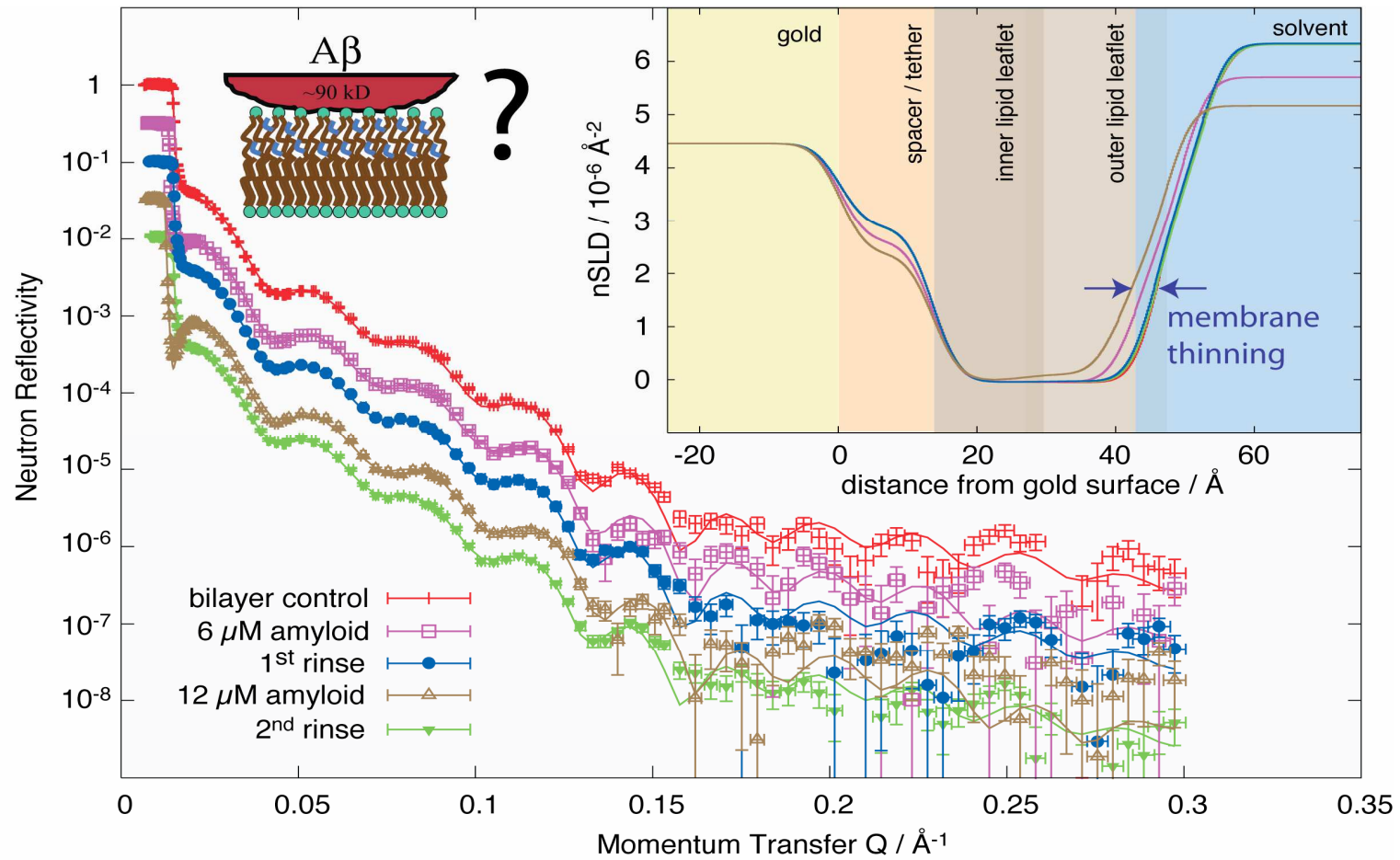
# Fit Robustness



9 best fits to a model



# Simultaneous Fitting

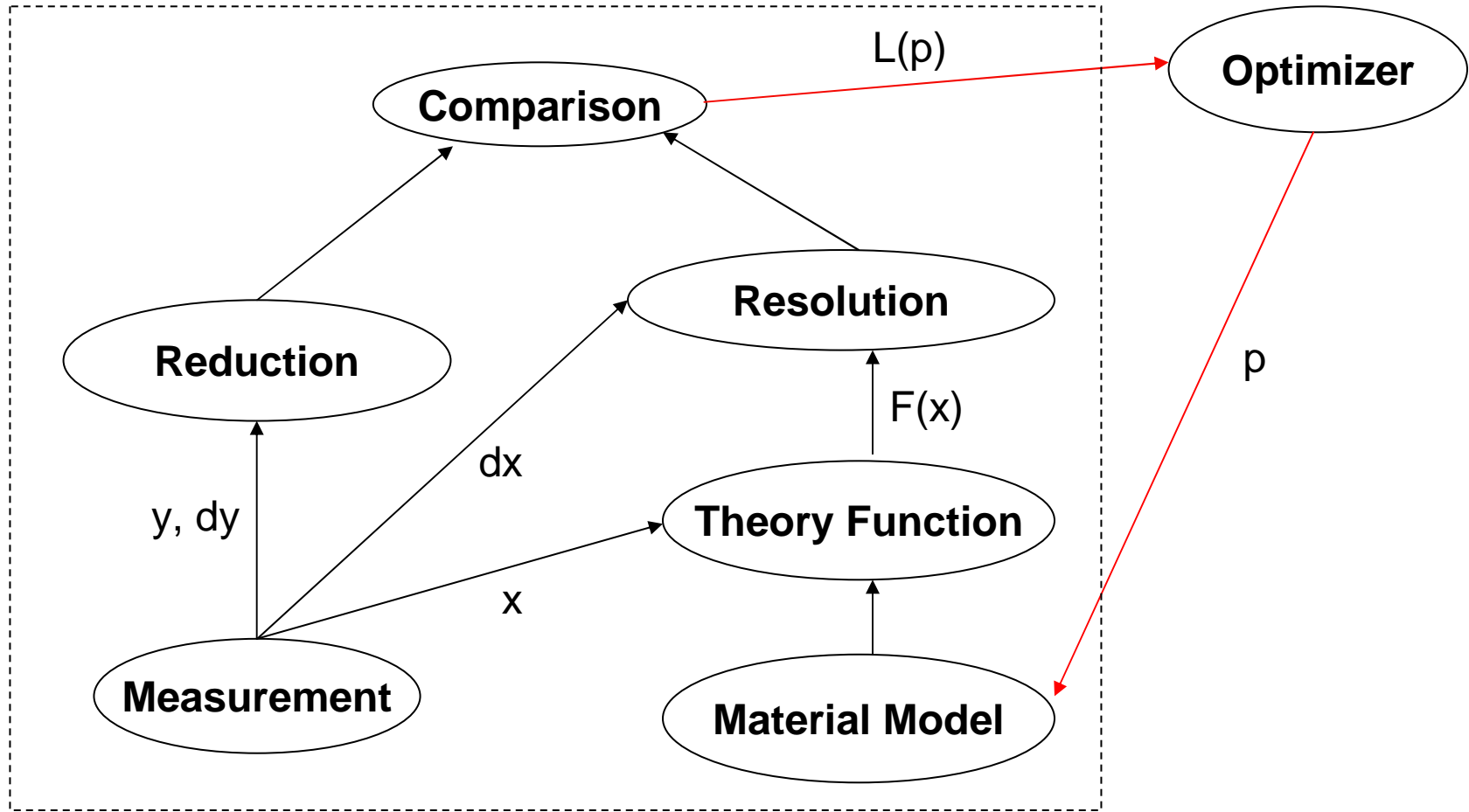


# Optimization Design Goals

- Constrained global simultaneous fitting
- Identify all good minima
- Ease of use
  - Track and compare completed fits
  - GUI client with interactive feel
  - Simple to install and maintain
- Parallel implementation for speed
- Extensible modeling environment



# Fit Function

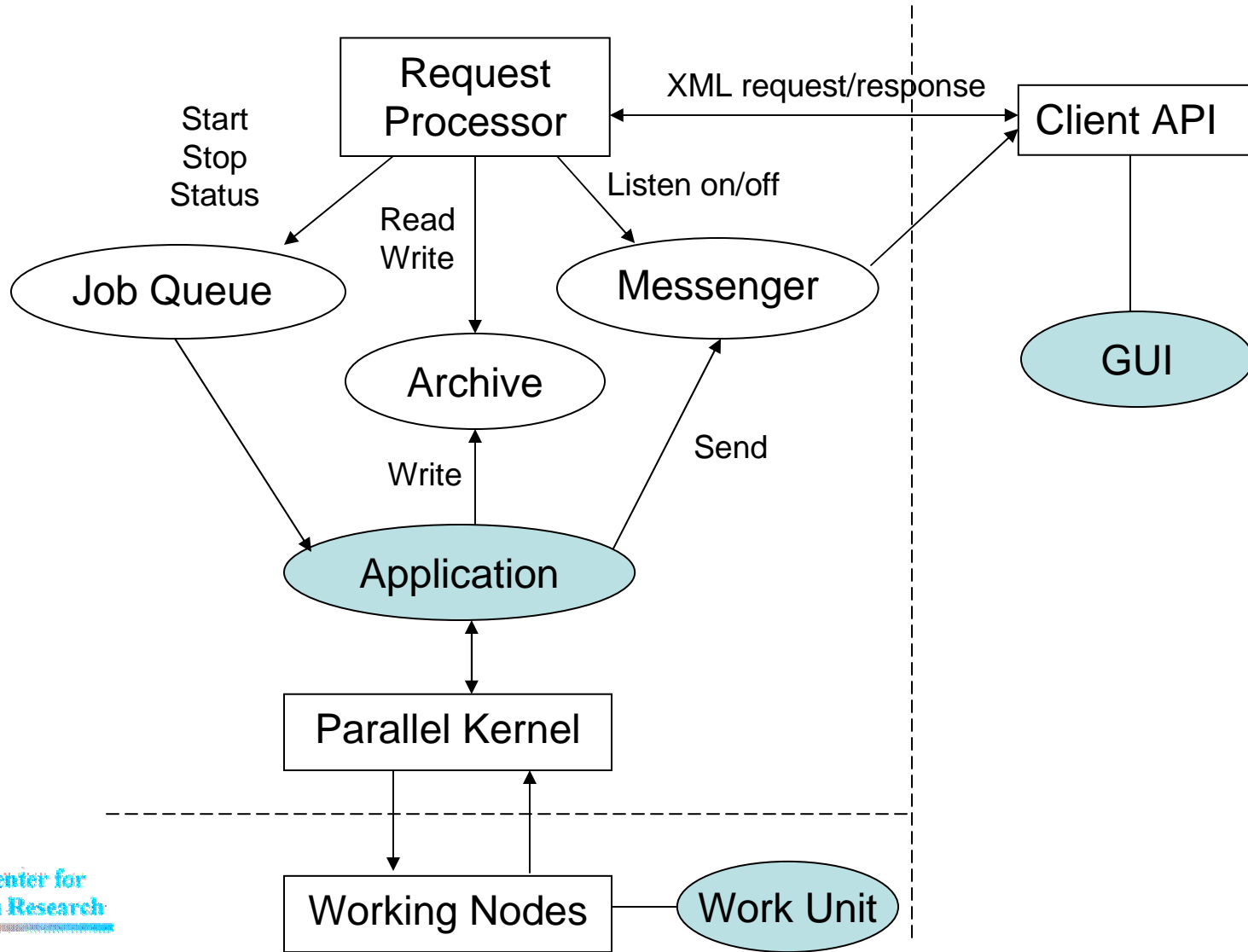


# Global Optimizer

- Simple algorithm:
  - Map local optimizer on model across  $n$  random starting points in the fit space
  - Reduce to parameter set with lowest value
- Large computation chunks reduce communication overhead
- Reduce function feeds improvements to UI
- Monte Carlo estimates for uncertainty



# PARK Service



# Map-Reduce

- Fault tolerant
- Self balancing
- Handles job priorities fairly
- Architecture neutral
- ...but...
- Embarrassingly parallel problems only



# Deployment

- Unconnected laptop
- University workgroup computers
- Facilities dedicated cluster
- CPU Harvester?
- Grid?



# Status

- Prototype parallel fitting (WBS 5.4.2)
- Prototype reduction code (WBS 9.1)
- Prototype 1D models (WBS 9.2)
- Constructed and measured 3D systems; started reduction and analysis (WBS 9.3)
- First results from 1D global simultaneous fitting with flexible modeling at MMM 2006
- Installing at SNS in early June



# Staffing

- Wenwu Chen
  - Fitting service
- Ziwen Fu
  - 1D Reflectometry modelling
- Christopher Metting
  - 3D Reflectometry modelling
- David Tighe (2007) and Alex Mont (2006)
  - Summer undergraduate students



End

