



Engineering Diffraction:

Project Status

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Outline



- Motivation
- Goals and Approach:
 - Ease of use
 - Materials model/theory integration
 - Forward experiment simulation
 - Inverse analysis of data
- Software and project update
- Personnel
- Education and outreach
- Future plans





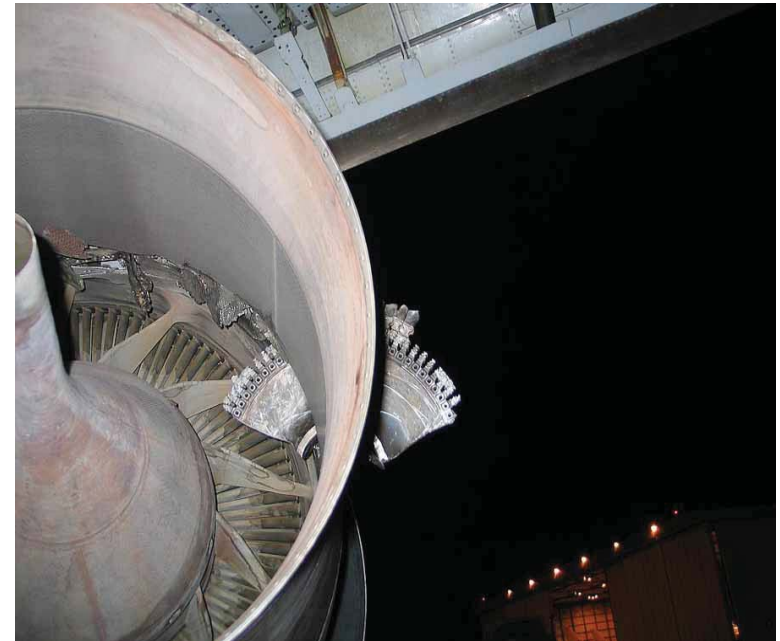
Motivation



How to predict performance and lifetime of engineering systems?



Petrobras, Brazil
(10 people killed, \$5 billion in losses)

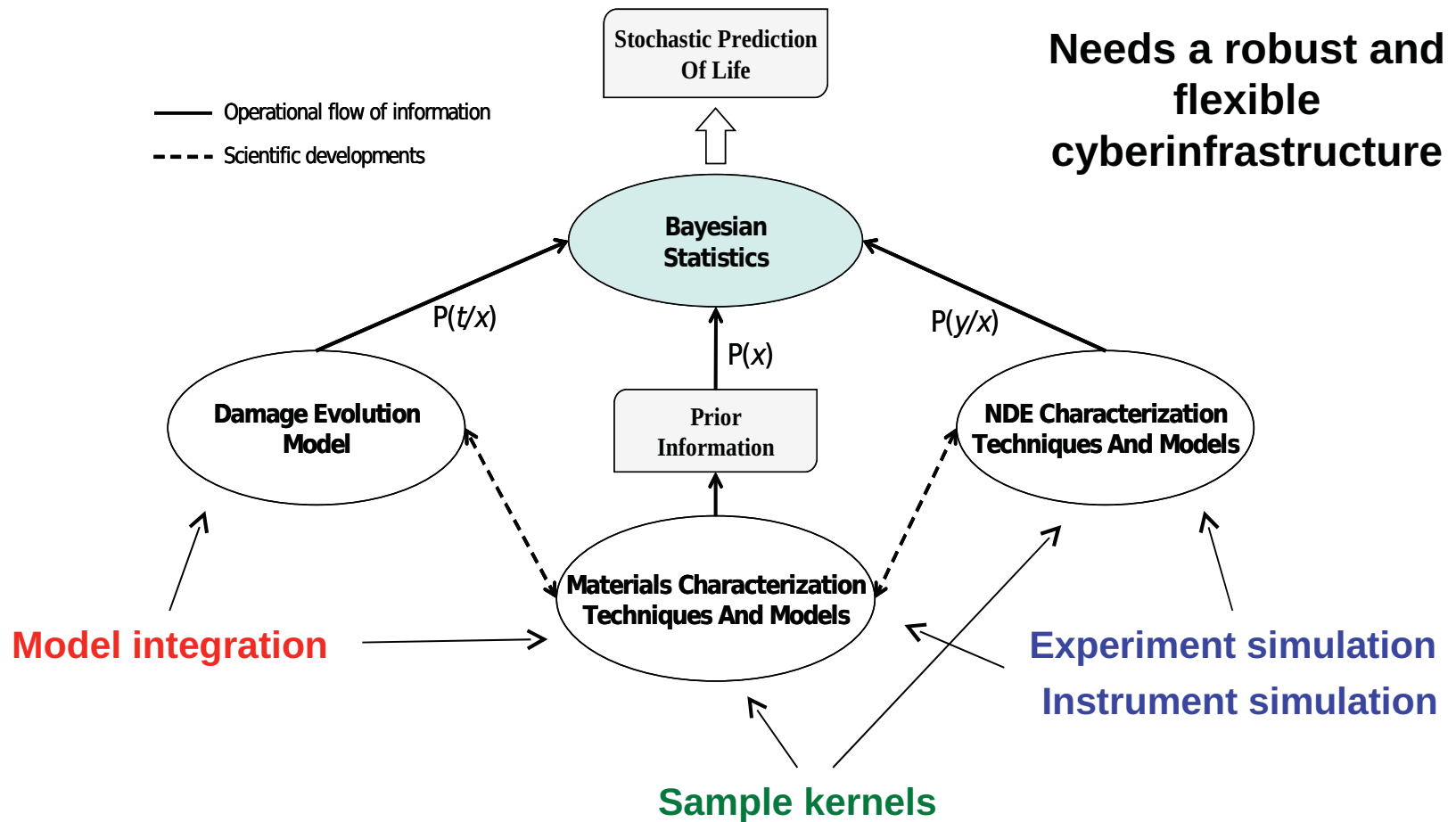


Turbine disk failure
(similar to the cause
of the Sioux City crash)





Motivation



Transformative change in engineering and materials fields





New *EngDiff* Science



- First study of dynamical diffraction effects in *EngDiff*
- First sample kernel that allows mechanical loading
- First to employ artificial neural network (ANN) analysis in *EngDiff*
- First rigorous inverse analysis in *EngDiff*
- New approaches to analyze anisotropic lattice strain data

Coming Soon:

- Flexible tools for coupled crystallographic and mechanics analyses
- Accurate calculation of *both* peak shape and position -> sophisticated experiment simulation
- Integration of advanced and multiscale materials models into experiment simulation
- Easy-to-use software, extensive documentation -> more output from *EngDiff* community





EngDiff Flagship Applications

- Mechanics Modeling:
 - *Cy-FEM* (Finite element modeling)
 - *Cy-SCM* (Self-consistent modeling)
- Experiment Simulation:
 - Sample kernels
 - Materials theory
- Data Monitoring and Analysis:
 - Real time data analysis
 - Texture analysis (*Cy-Tex*)
- Expert System:
 - ANN (artificial neural networks)
 - User guidance





Cy-SCM: Self-Consistent Modeling with EPSC



Cy-SCM (EPSC)

File Phase Optimization Run View Help

Active Data

- Model
- Experiment
- Optimization

Plot Options

Macro

- Model Result
- Experiment Data

Neutron

- Model Result
- Experiment Data

Plot Reset

Ready

6

ε

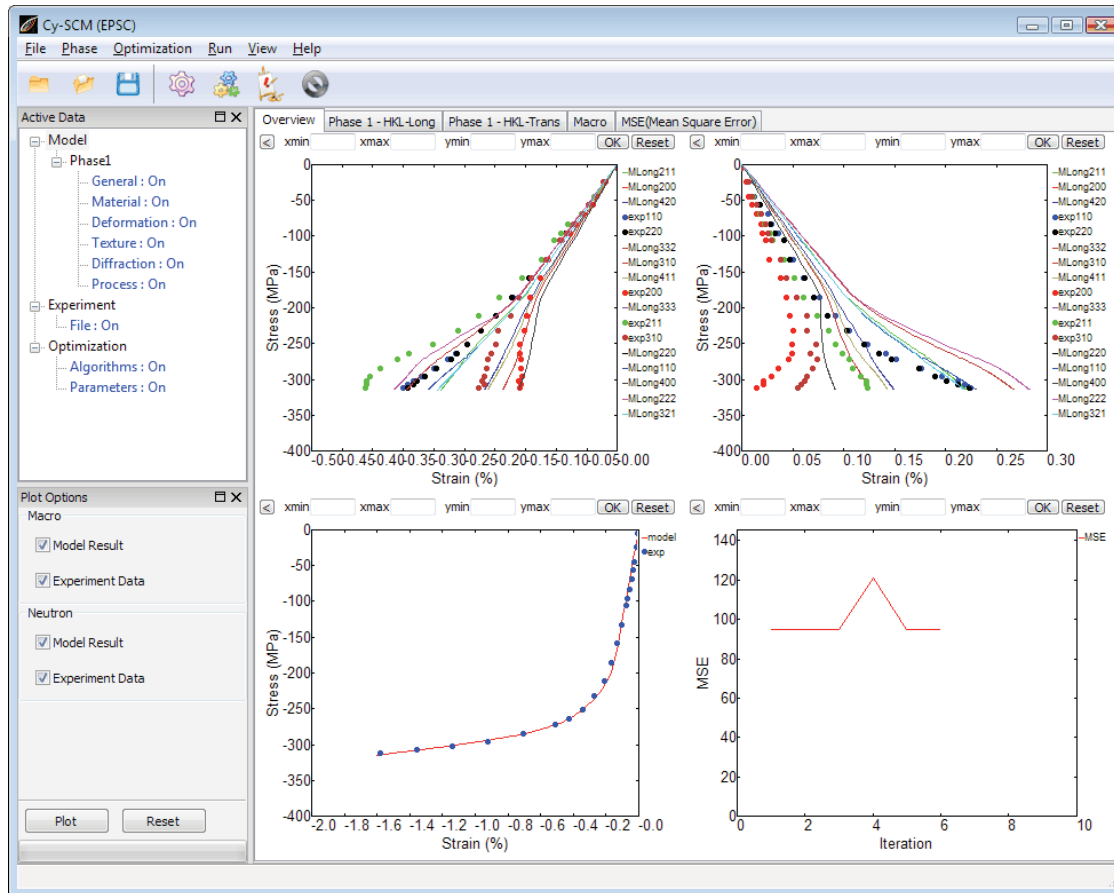
Cy-SCM
Version 1.0 Alpha

Self Consistent Modeling for Engineering Diffraction
Iowa State University





Cy-SCM: Self-Consistent Modeling with EPSC

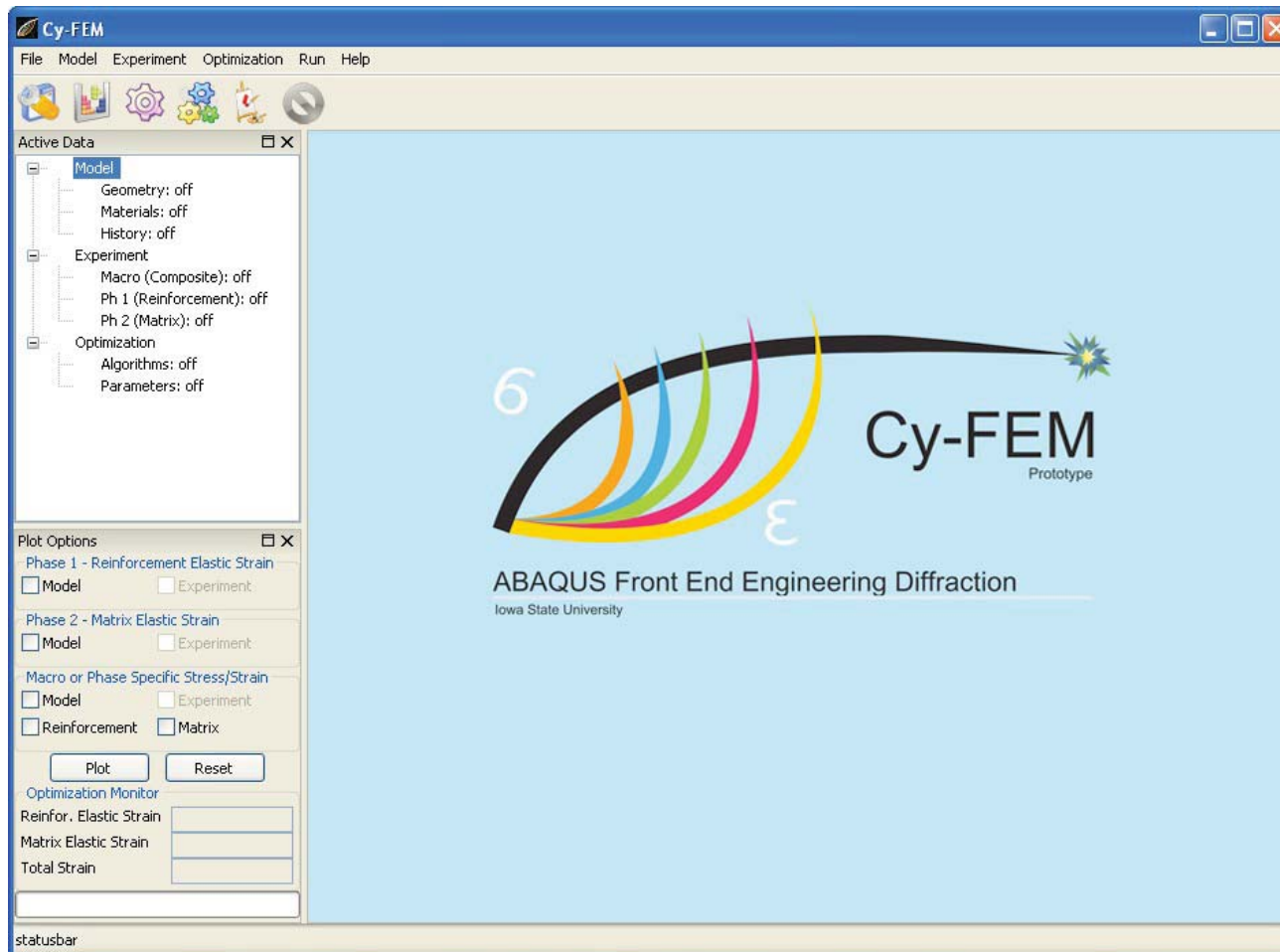


- Integrated EPSC into DANSE framework
- Allowed optimization of hkl data as well as macro strain data
- Streamlined data I/O
- Significantly improved user friendliness
- Enhanced calculation speed
- Introduced optimization algorithms
- Defined a new cost function
- Designed baseline for future improvement of the SCM:
 - Integration of other SCM models (VPSC, ferro-SCM, etc.)
- Allowed simultaneous optimization of multiple datasets





Cy-FEM: Finite Element Analysis with ABAQUS



- Integrated ABAQUS into DANSE framework
- Streamlined data I/O
- Significantly improved user friendliness
- Introduced optimization algorithms
- Started a sample geometry library:
 - Fibrous and particulate composites
 - New ones to be added
- Allowed simultaneous optimization of multiple datasets





Instrument Simulation & Support



New sample kernels to simulate experiments:

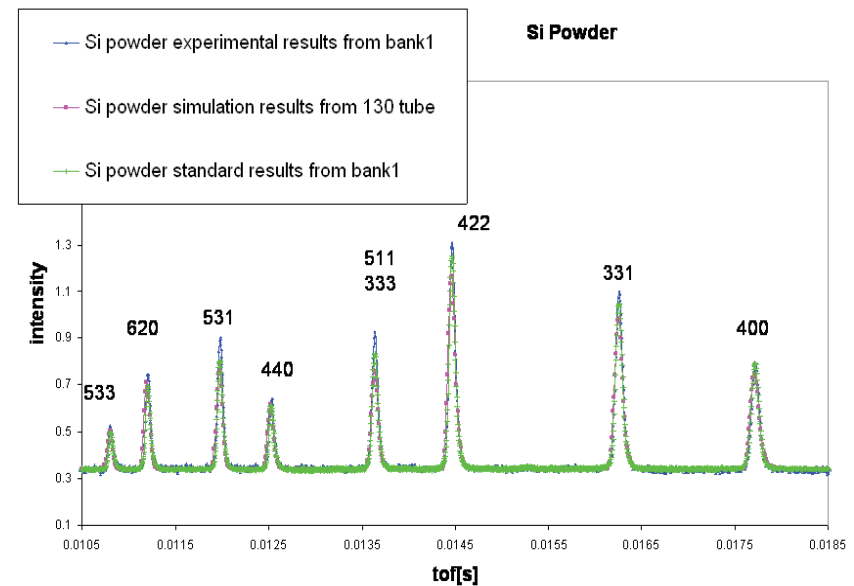
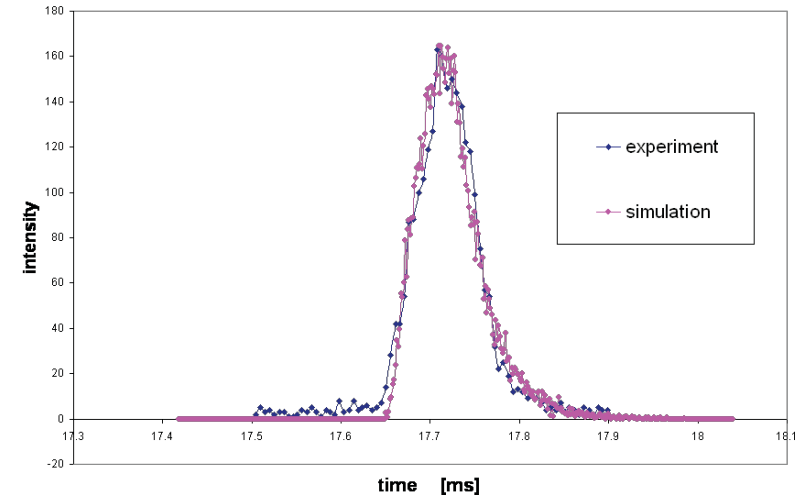
- Powders
- Single crystals
- Polycrystals under load

Crucial foundation for sophisticated microstructure simulation

Integration into VNF underway

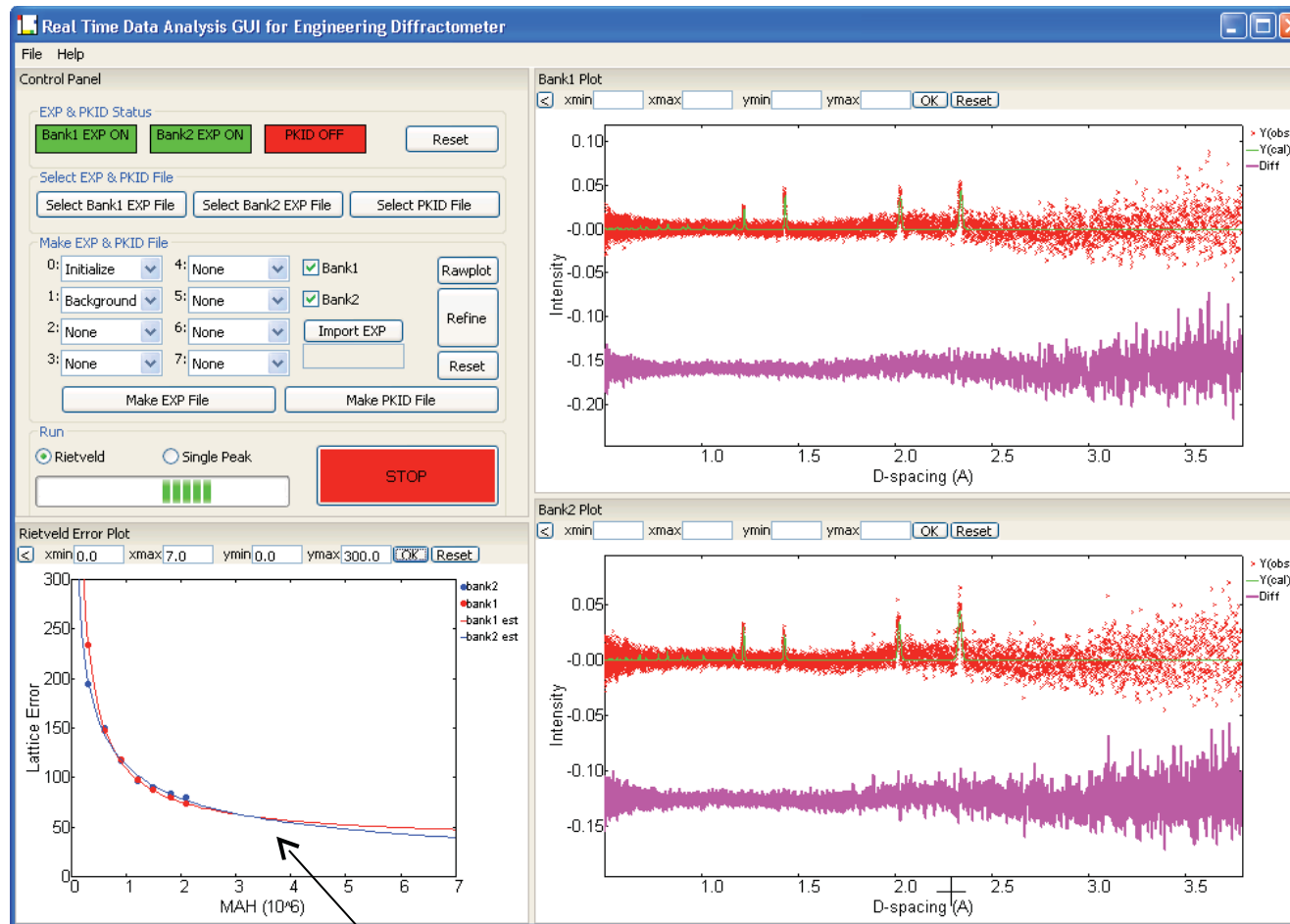
SMARTS and HIPPO simulations almost ready

VULCAN simulation in late 2009
(Also influenced VULCAN design)





Real Time Data Analysis



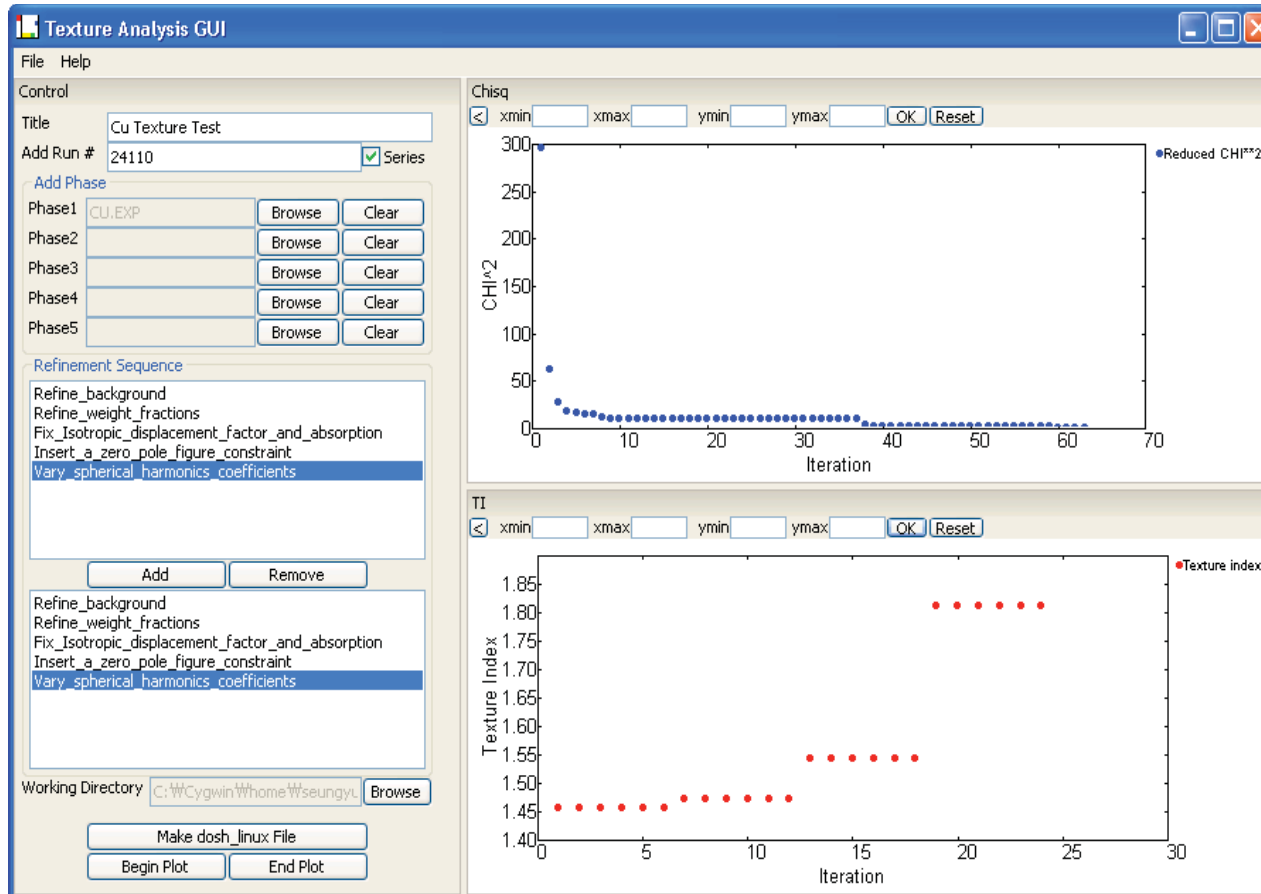
Monitoring of measurement error

- Reduces raw data
- Performs quick data analysis:
 - Rietveld refinement
 - Single peak fitting
- Updates every 30 sec
- Helps user monitor progress of exp.
- Crucial for beam time optimization
- To be used at Lujan Center on SMARTS and HIPPO in Summer 2009





Cy-Tex: Texture Analysis



- First time integration of multiple texture tools
- Runs legacy code (GSAS, MAUD, popLA)
- User friendly
- Communication with mechanics and materials models
- Flexible for future growth
- To be used at Lujan Center on SMARTS and HIPPO in Summer 2009
- Crucial for Geophysics community





Artificial Neural Network (ANN) Application



The screenshot displays the EngDiff software interface with several windows open:

- ANN training:** A window showing training parameters (e.g., 3028 iterations, 500 testing iterations) and a plot of Mean Squared Error (MSE) vs. Iteration/10, showing a sharp decrease in error over time.
- Artificial Neural Network (ANN) Prototype:** A window with two plots: "Fiber Lattice Strain" and "Total Composite Strain". Both plots show Applied Stress (MPa) vs. Strain, with red dots for imported data and blue lines for simulated data.
- Inverse Analysis Prototype for Uniaxial Fiber Composite Model via ANN Forward Engine:** A window with two plots: "Fiber Lattice Strain" and "Total Composite Strain", similar to the ANN Prototype window.
- Properties:** A window showing material properties for Fiber and Matrix, including Young's Modulus (GPa), Tau Zero (MPa), Tau One (MPa), Theta Zero (TPa), Theta One (GPa), and Yield Strength (MPa).
- ANN Forward Run:** A window with optimization settings (e.g., Fiber Elastic, Total Composite) and optimization algorithms (ANN Inverse Model, leastsq, DE1, DE2, Snobfit).
- ANN inverse model:** A window showing overall and fiber properties, including Fiber Volume Fraction, Initial Processing Temperature, Matrix Young's Modulus, Matrix Properties and Constitutive Law (Power-law) Parameters, Yield Strength, and Power Law Coefficient.

- First time use of ANN in *EngDiff*
- Extreme improvement in forward model calculation speed
- Can be adapted for other models





Release and Deployment Schedule



- *Cy-SCM*: alpha version released
- *Cy-FEM*: prototype released
- Real time data analysis: to be used at LANSCE in 06/2009
- Texture analysis: to be used at LANSCE after 06/2009
- SMARTS and HIPPO simulation: later in 2009
- VULCAN simulation: late 2009





Personnel Update



- Current team:
 - Seung-Yub Lee: lead developer
 - Youngshin Kim: developer
 - Hyuntae Na: graduate student
 - Goknur Tutuncu: graduate student
 - Sarah Ross: undergraduate student
 - Li Li (Columbia): graduate student
- Two very capable developers left early (M. Motahari and A. Mahajan)
- New grad student (H.T. Na) started in Jan. 2009 and has been highly effective
- Budget cuts (\$150k–15%) hampered efforts for earlier hiring
- New developer(s) to be hired soon





Education and Outreach



- Undergraduate students:
 - 5 total; 2 female; 1 paper in preparation
- MS thesis completed (B. Denizer)
- Female developers:
 - Y.S. Kim and G. Tutuncu
- Close collaboration with LANSCE:
 - Use of code on SMARTS and HIPPO
- Use of *EngDiff* code in teaching:
 - MatE-418: *Cy-FEA* (34 students)
 - MSE-540: *Cy-SCM* (15 students)
- Support for **Geophysics** community (SCM and texture analyses)





Future Plans



- Task re-baselining in progress
- Materials theory work to increase soon:
 - Dislocation dynamics (LeSar)
 - Realistic microstructure (LeSar)
 - 3-D FEA (Dawson)
- Improvements in *Cy-SCM*: VPSC, ferro-SCM
- Close collaboration with LANSCE to continue
- VULCAN deployment to start in late 2009





Issues



Please inquire to Mike McKerns or Brent Fultz for access to information contained in this slide.

