

DANSE Fitting Service

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DANSE WORKSHOP

SNS

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Objective

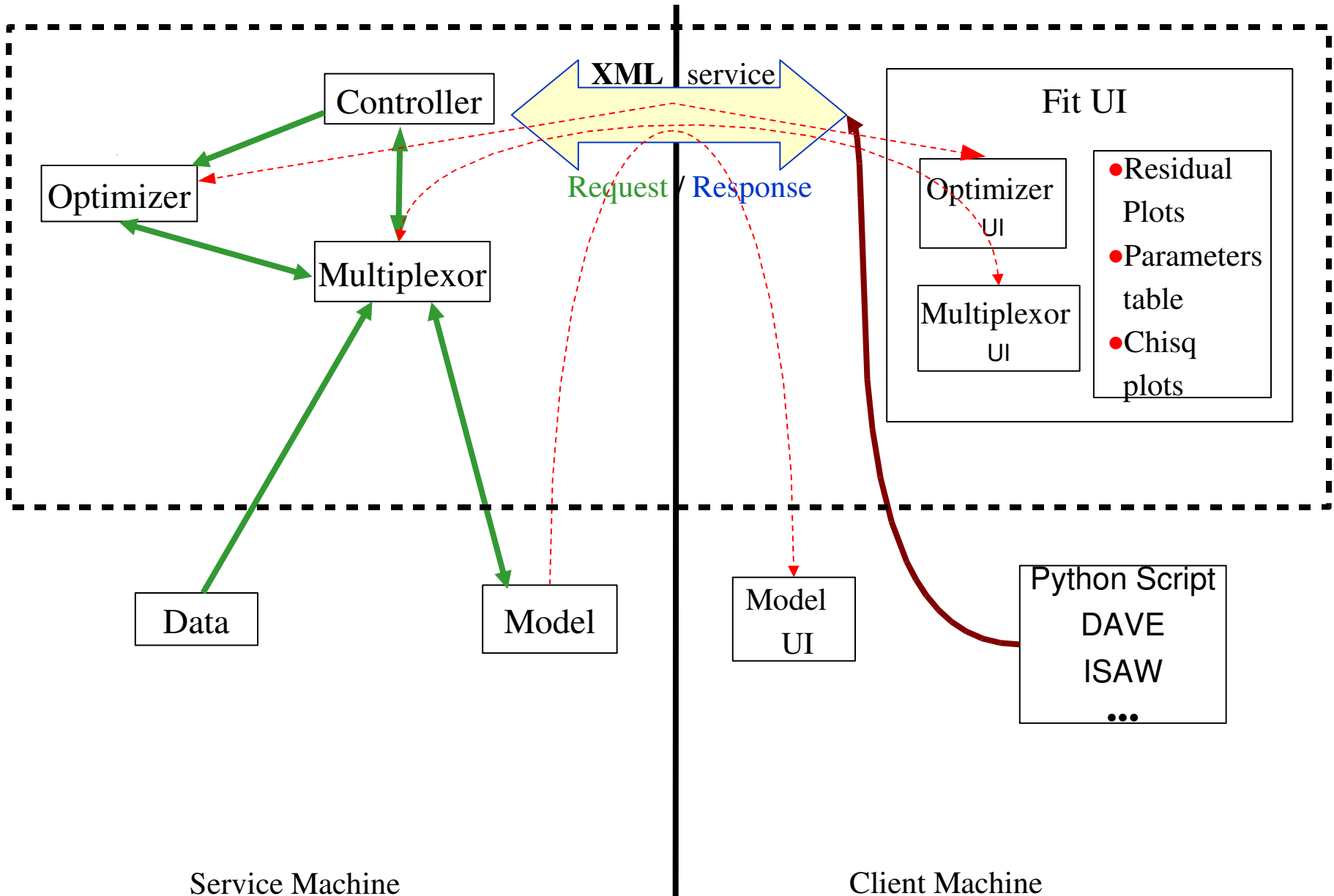
- DANSE fitting service
- multiplexor (for simultaneous fitting)
- parallel architecture
- other reflectometry projects

Fitting Requirements

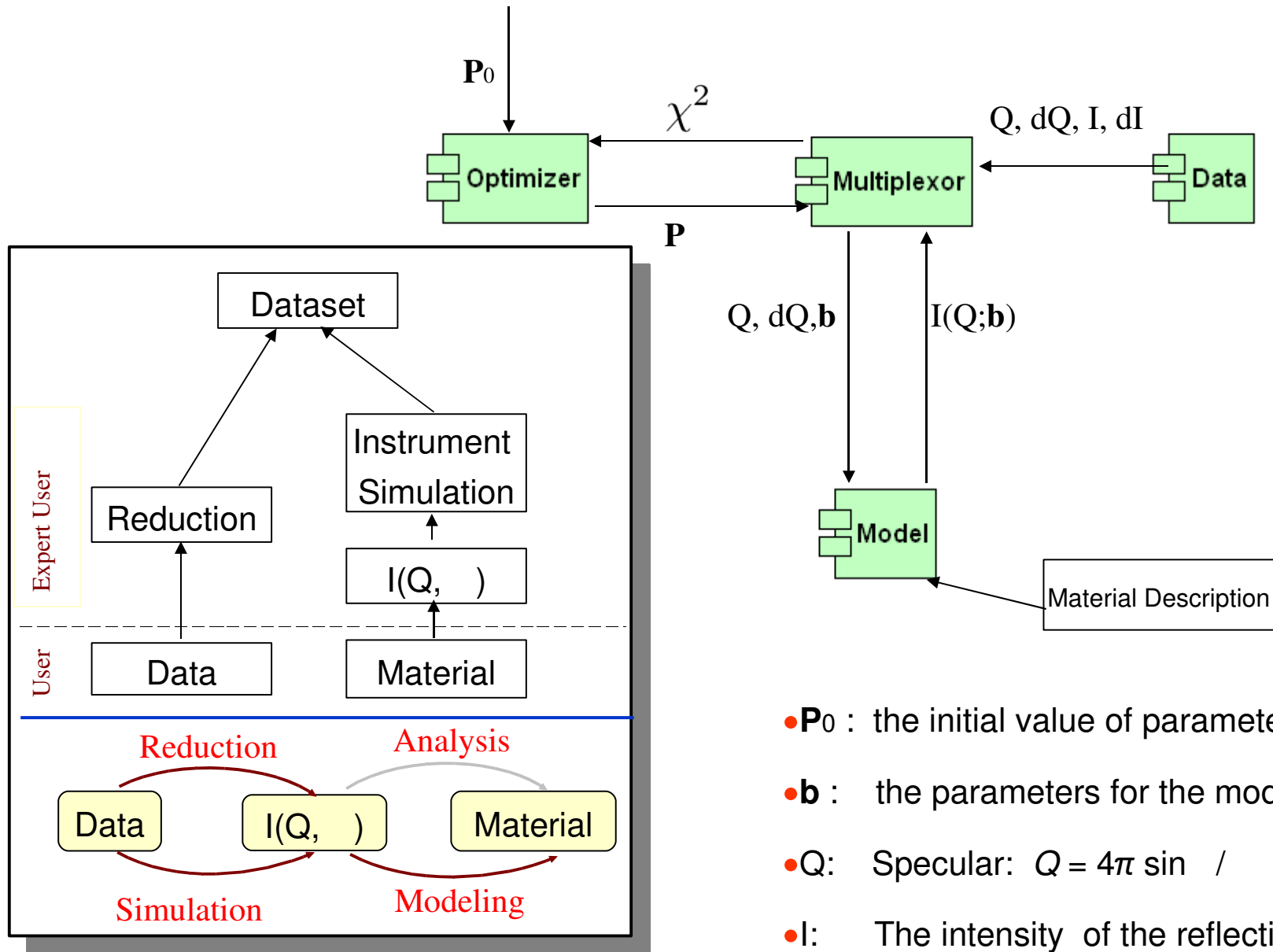
- **Problem space**
 - **global derivative-free constrained fitting**
- **Data manipulation**
 - **reduction and simulation steps**
- **Reliability and confidence**
 - **indications of confidence in the fitting results**
- **Usability**
 - **model specification and workflow**
- **Deployment**
 - **single user, university group, national labs**

See: <http://danse.us/trac/tickets/wiki/BasicOptimization>

Fitting Service



What is the Model?



Multiplexor

Optimization Vector

2.549
8.631
27
...

Parameter Table

	Attribute
P1	=P2
P2	▶ [3,4]
P3	0
P4	-0.56
...	...
	▶ 8.631
	▶ 27

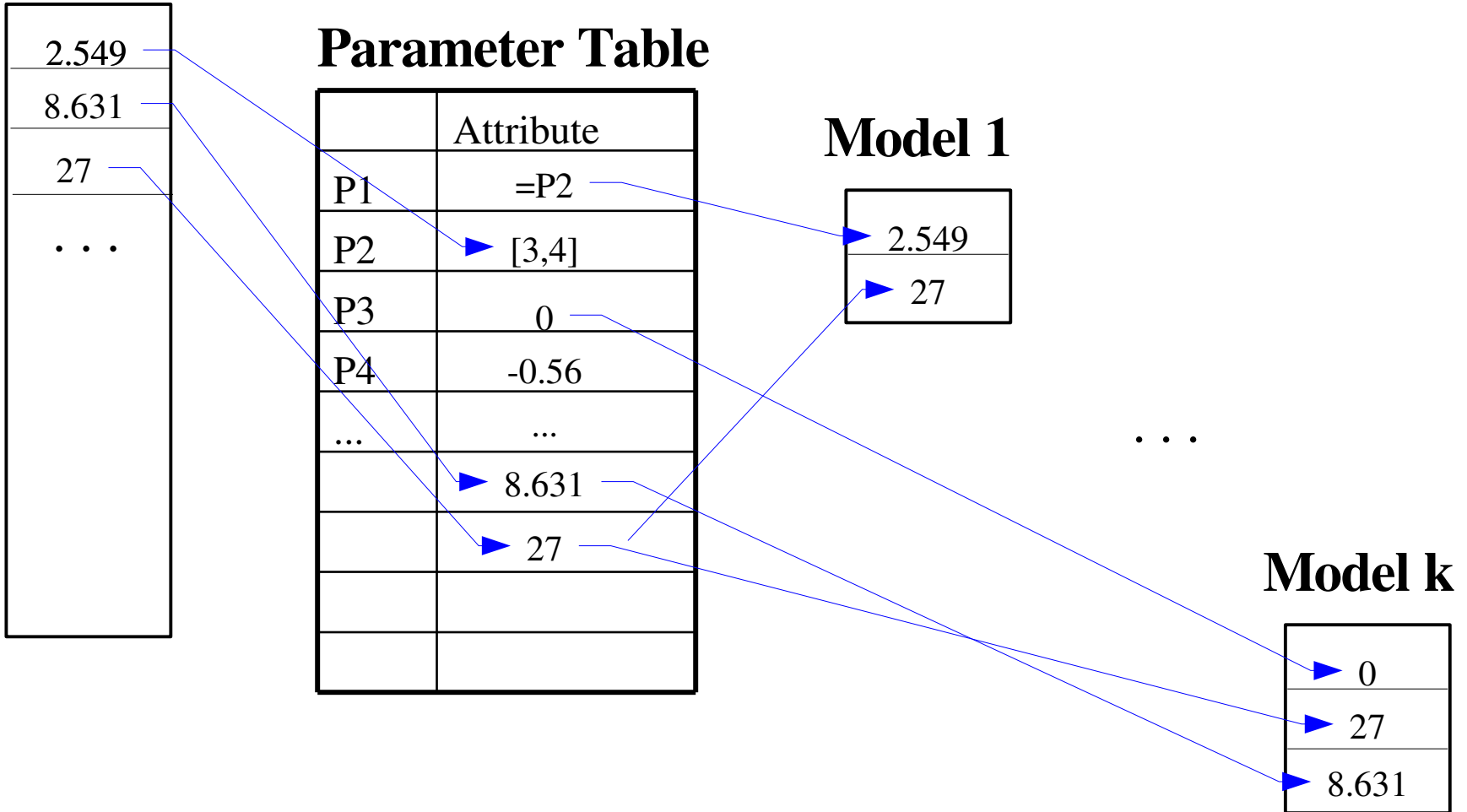
Model 1

2.549
▶ 27

...

Model k

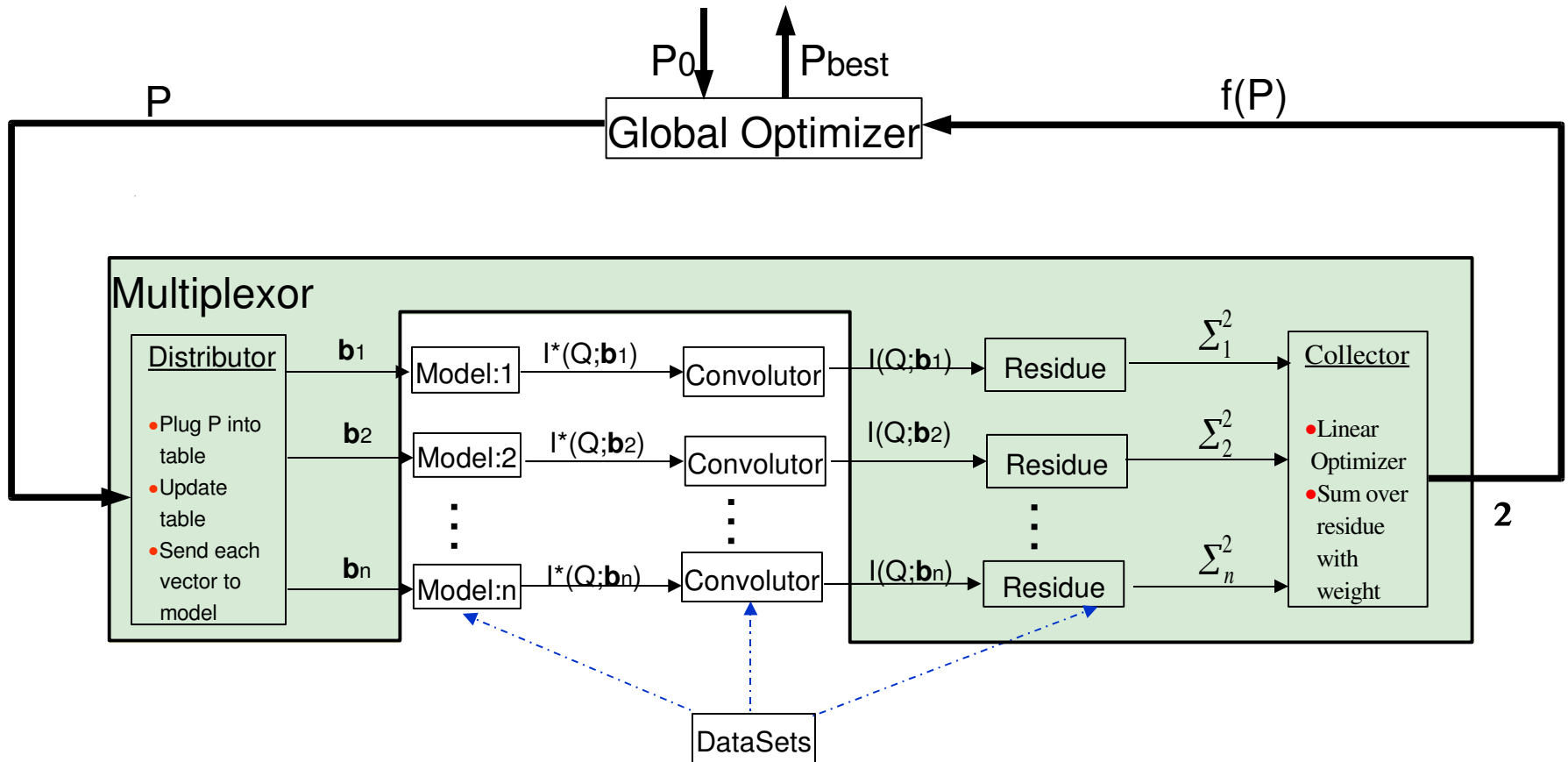
▶ 0
▶ 27
▶ 8.631



Multiplexor Pseudocode

- Receive \mathbf{P} from global Optimizer (initially \mathbf{P}_0), containing only the varying parameters.
- Substitute \mathbf{P} into value table.
- Evaluate relations between parameters
- Extract model Parameters from value table
- Call Model i with \mathbf{b}_i to evaluate $f(\mathbf{b}_i)$
(including the instrumental effects)
- Feed into linear optimizer and
return 2 to global Optimizer

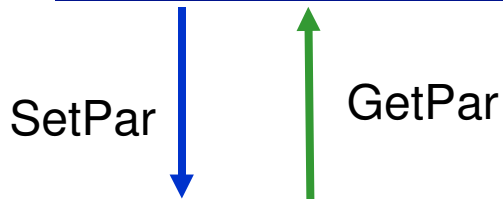
Multiplexor Dataflow



- User can set up weights from UI
- Some of the parameters in b_1, b_2, \dots, b_n are common parameters

Multiplexor UI

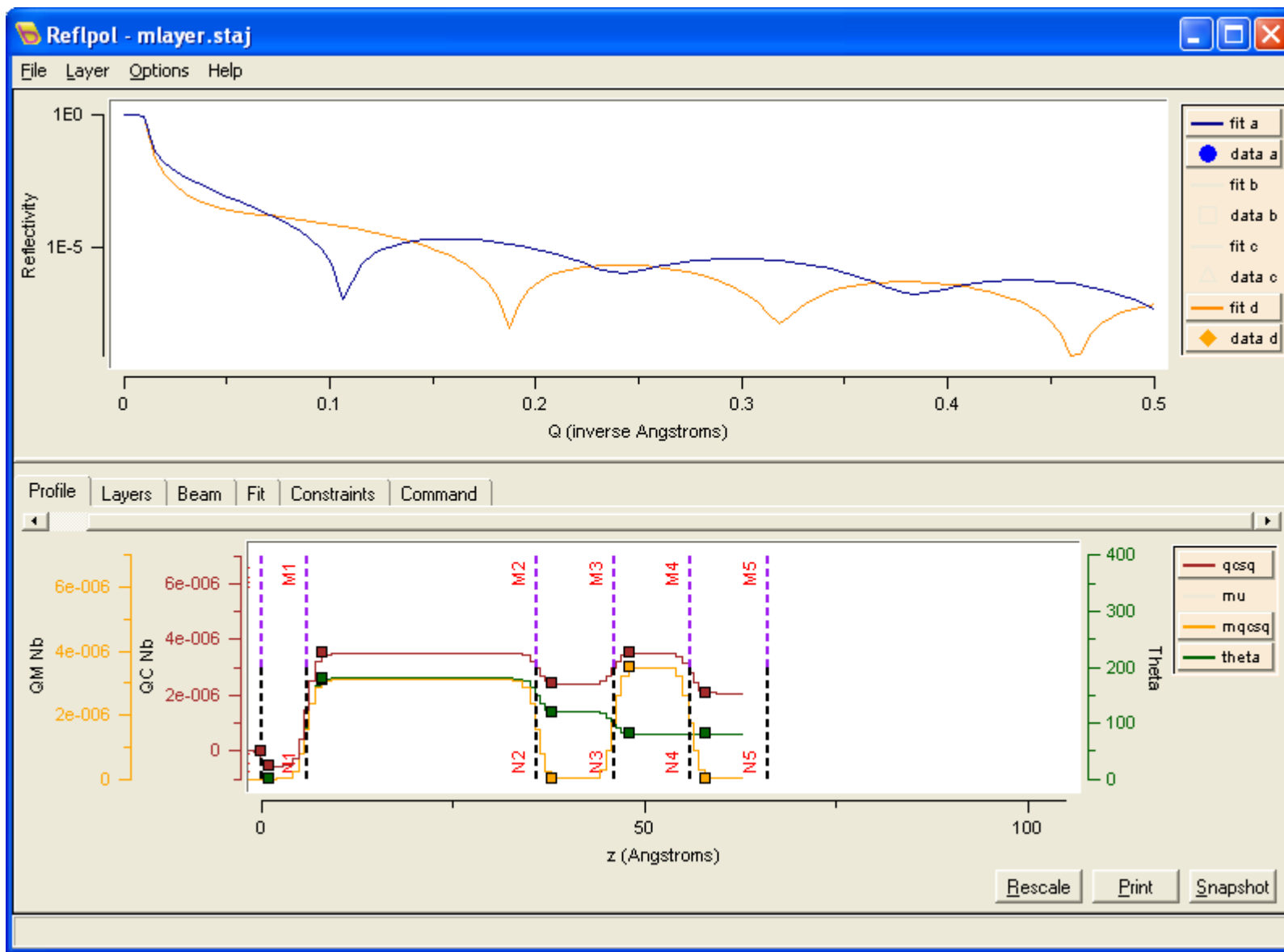
	A	B	C	D	E	F	G	
1		thickness	SLD	MagneticSLD	Angle	Layer	Magnetic	Ang
2	Air		0			=Infinite(C2)		
3	IrMn	0.6	-0.56			=flat(B3,C3)		
4	CoFe	3	[3,4]	[0,5]	[0,360]	=flat(B4,C4)	=spline(5,E4)	=spline(5,E4)
5	Cu	1	2.4			=flat(B5,C5)		
6	CoFe	1	=C4	[0,5]	[0,360]	=flat(B6,C6)	=spline(5,E6)	=spline(5,E6)
7	Si		2.07			=Infinite(C7)		
8	Model	=magnetic_reflectivity(F2:F7,,G2:G7,I2:I7)						



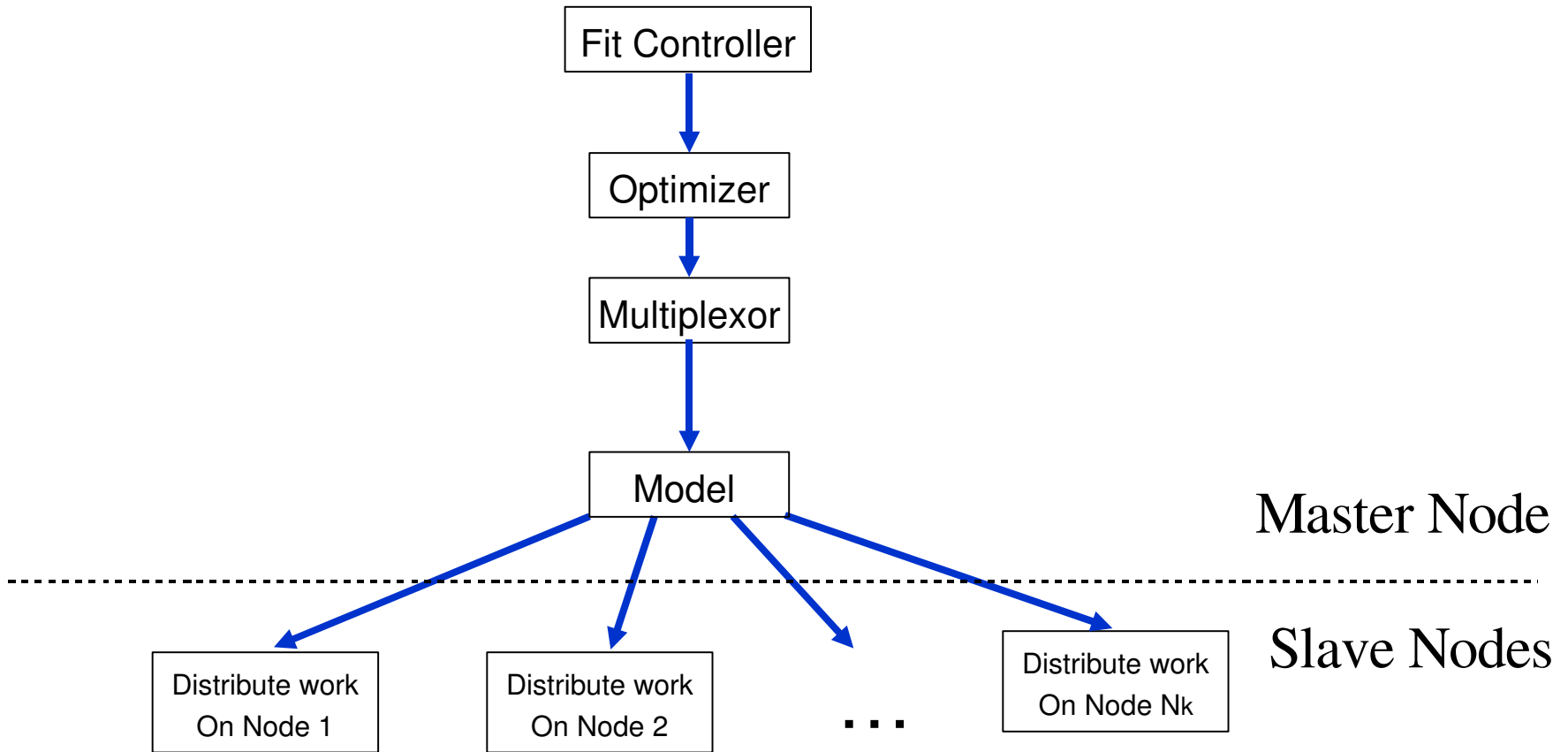
		Attribute
C6	P1	=P2
C4	P2	[3,4]
C2	P3	0
C3	P4	-0.56
...

- Spreadsheet for generic model UI
- Supports ad hoc calculations without programming
- Cells may contain DANSE components
- Data files associated with spreadsheet
- Attribute including: low, hi, uncertainty, constant, etc
- Templates for specific types of models (volume fraction, magnetic, polymer, ...)

Model UI

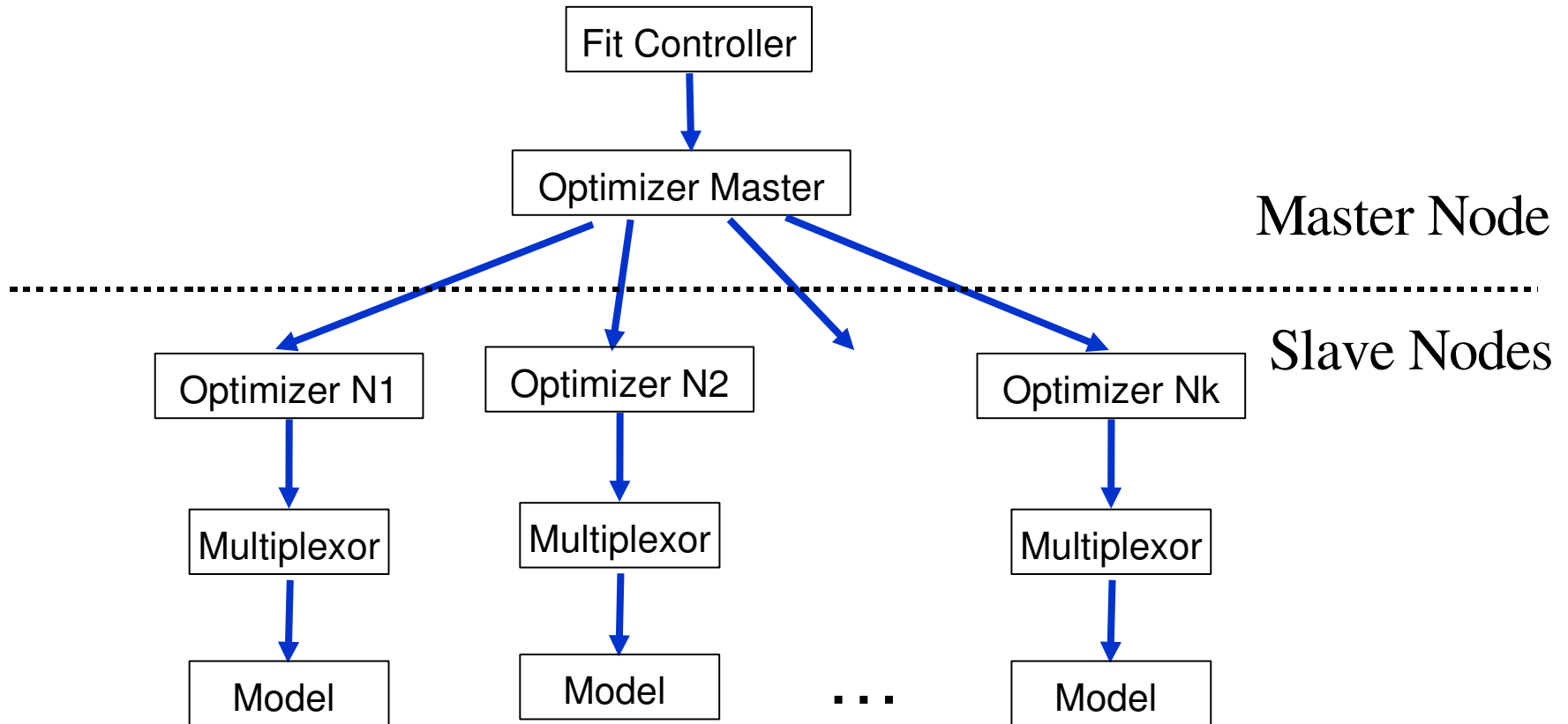


Parallel Model



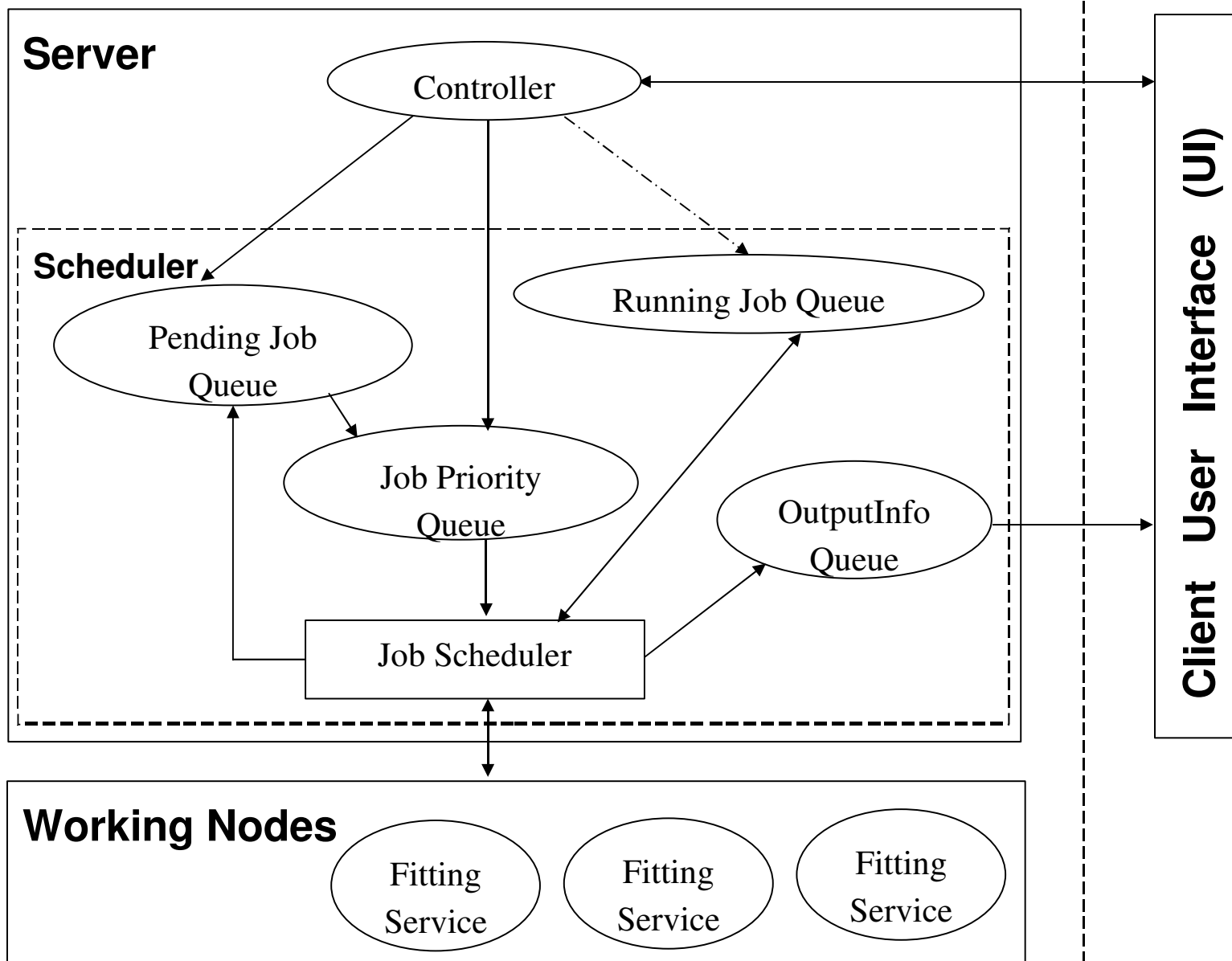
- Parallel CPU on Node 1 (N1), Node 2(N2) , ..., Node k(Nk).
- In this Case, we parallelize the Model, For example, In MD simulation.

Serial Model



- Parallel CPU on Node 1 (N1), Node 2(N2) , ..., Node k(Nk).
- In this Case, we parallelize the Algorithm for Optimizer.

Server Architecture



Other Projects

- **Data viewing/reduction**
 - extending reflpak to handle TOF data
 - defining NeXus format for reflectometry
- **Off specular reflectivity**
 - defining parameters of interest
 - acquiring and measuring patterned samples
 - investigating existing GSAXS software
- **Testing prototype on complex models**
 - 10 layer magnetic system, possibly with twist
 - fitted with KsRefl (to appear in IEEE TransMag)

Reflectometry Team

- P. Kienzle (NIST)
- Z. Fu and W. Chen (NIST/U Maryland)
- C. Metting (U Maryland)
- A. Mont (U Maryland)
- C. Majkrzak, *et al.* (NIST)
- J. Ankner, *et al.* (SNS)