

# **Laboratory Information Management System**

## **Designing a LIMS for the BBSRC SPoRT Initiative**

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Robert Esnouf, Anne Poupon, David I. Stuart, Chris Morris**



# This Talk

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- **Overall Theme**
- **Management**
- **Software Architecture considerations**
- **Interoperability & OMG**
- **Workflow**
- **What's it got to do with a beamline**

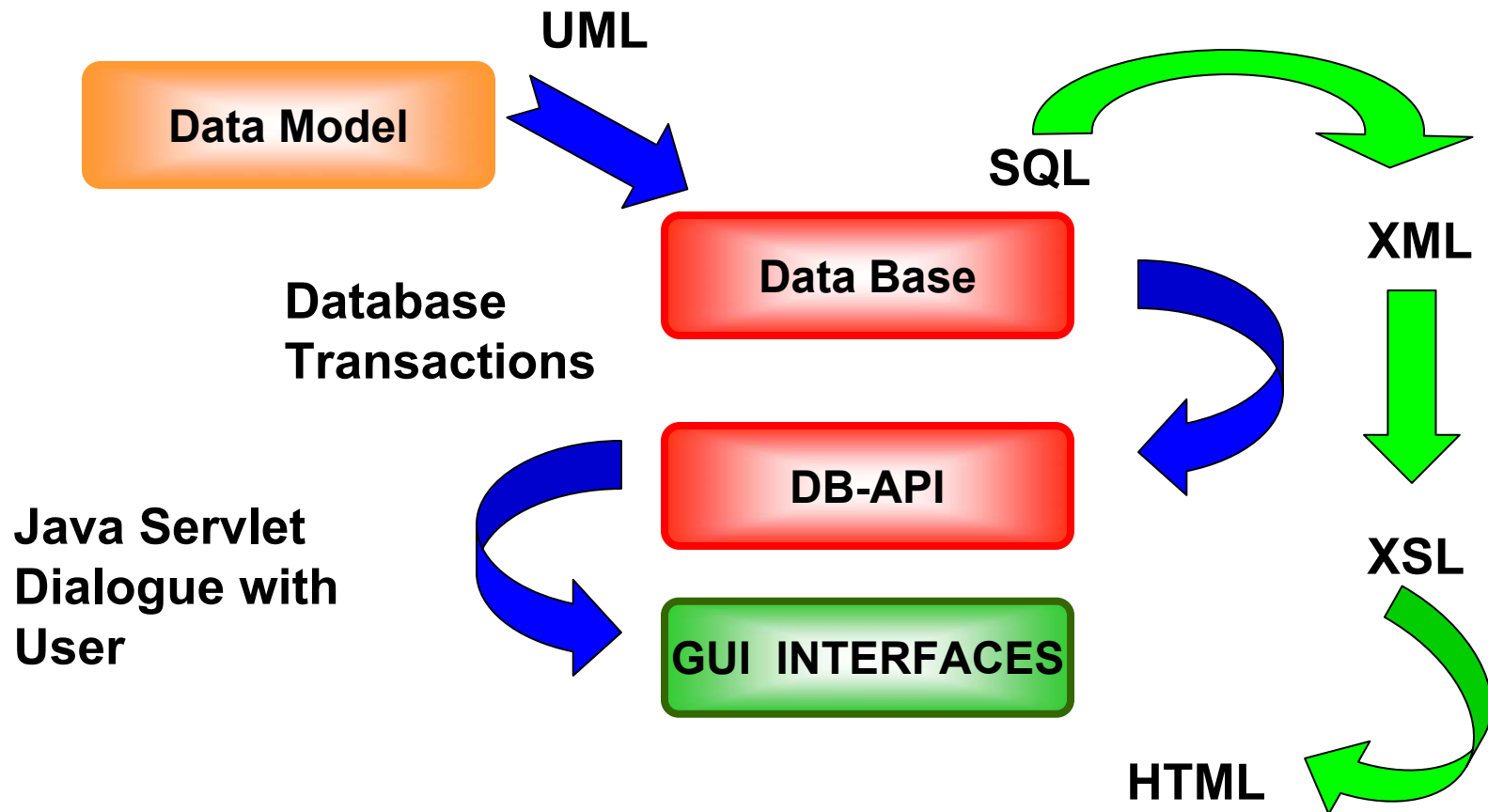
**We are not:**

- OO experts**
- UML experts**
- Early adapters of anything**

**We are:**

**Keenly interested in improvements**

# LIMS Modular Construction



## DB-API

The key, top-level components of the LIMS API are:

- **To describe Work at a high level**
- **To describe Work at a low level**
- **Classes to represent the Materials.**
- **Classes to implement the Work.**
- **Classes which record the Work results.**
- **A Work Engine**
- **A Storage Engine**

BI

**Web server**

**Generic  
User  
Interface**

**Specific User Interface**

**API for Laboratory Operations**

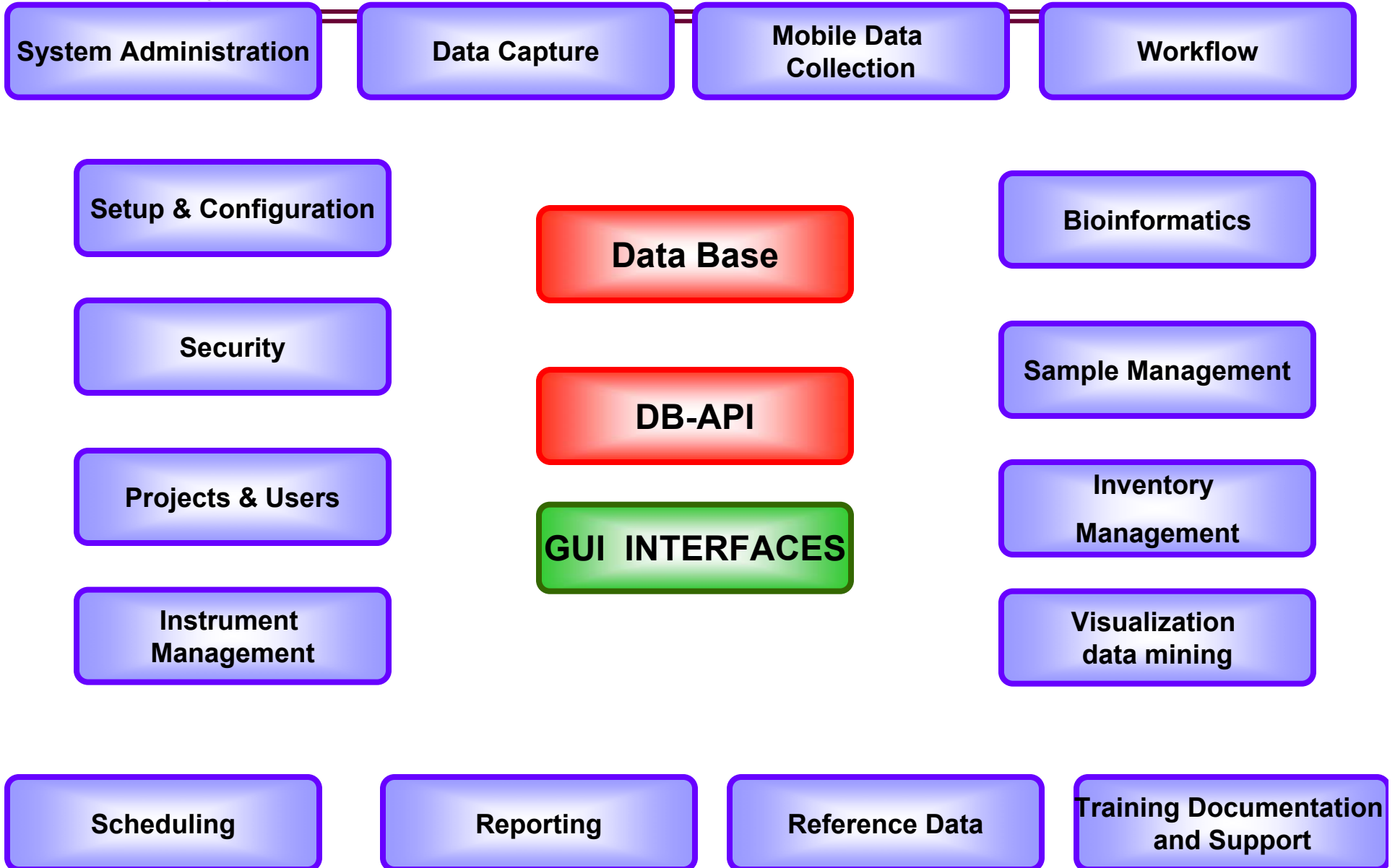
**Data model API (strongly typed)**

**Data access API loosely typed, supports metadata queries**

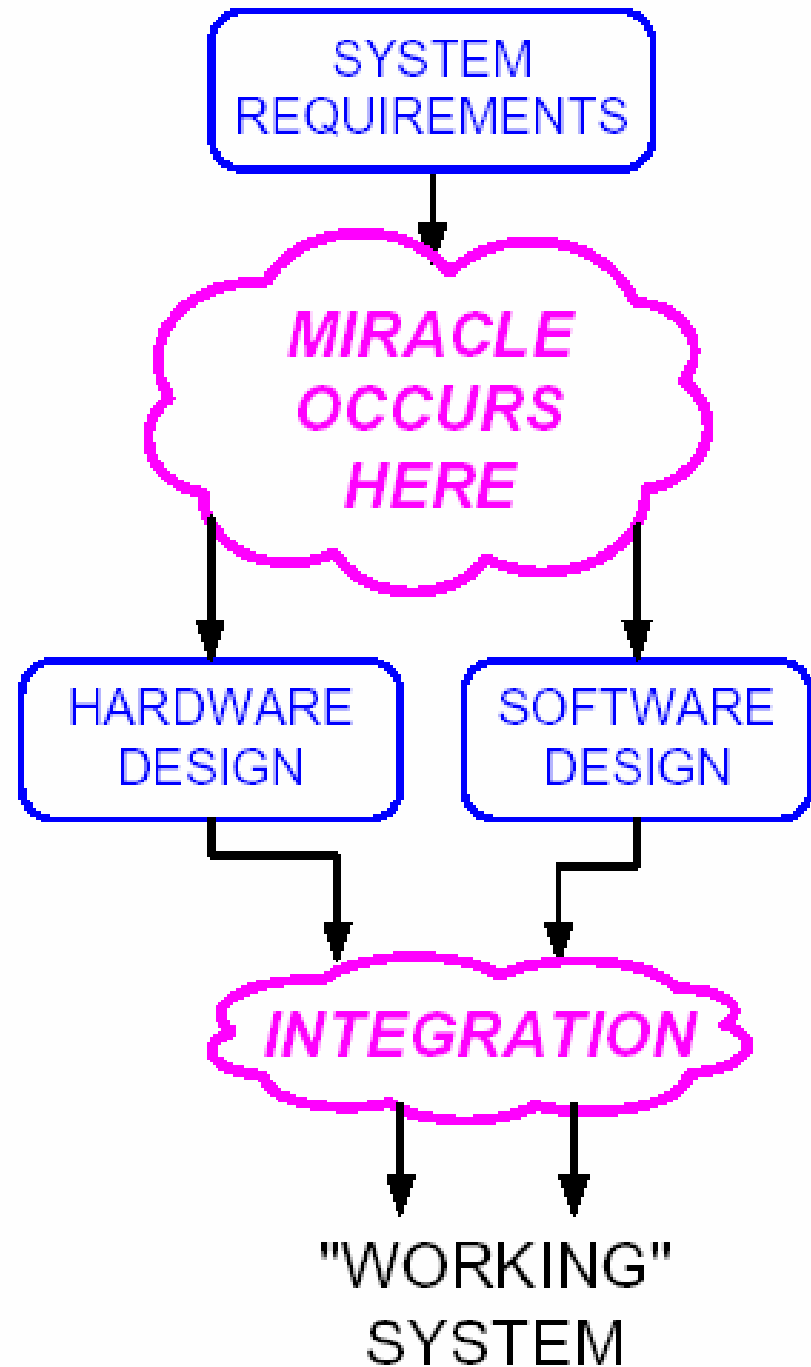
**Database**



# Modular Construction



# “Business Modelling and UML – Hype vs. Reality”





Colin Thurston  
Regional Sales Manager

# Scary Statistics

Only 9% of large IT projects  
are on time & on  
budget

31% of IT projects  
are cancelled before  
completion

52% of IT projects  
cost twice the  
initial budget to  
complete



# Project Management

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**All Projects have competing constraints**

➤ **Time, Costs and Functionality**

**Constraints management – key to success**

➤ **Must Have**  
➤ **Should Have**  
➤ **Could Have** } **MoSCow**

**Some requirements may slip to meet constraints**

**Pareto Principle**

➤ **80% benefit achieved with 20% of effort**

# Architecting a dog house

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**Can be built by one person**

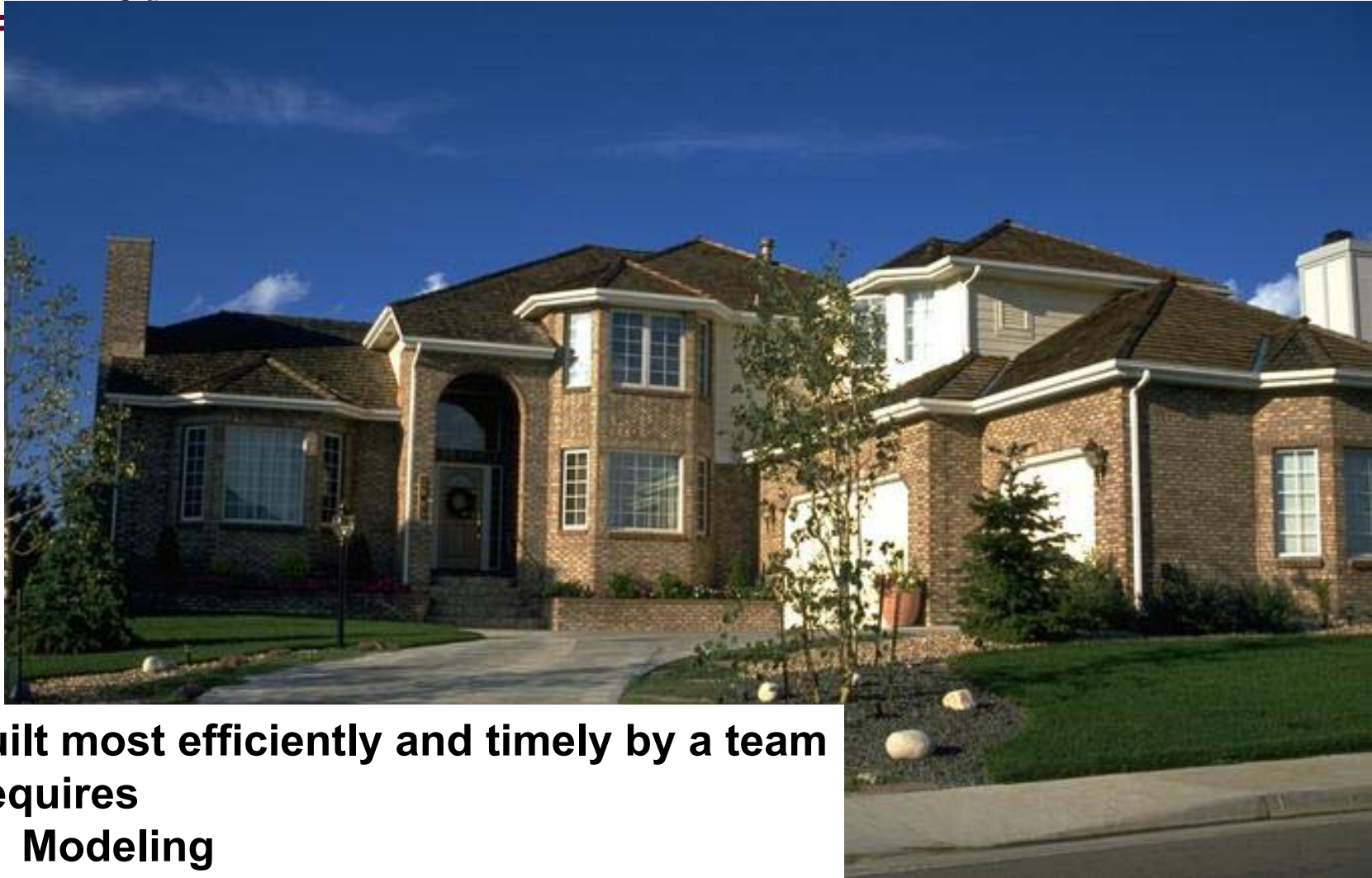
**Requires**

**Minimal modeling**

**Simple process**

**Simple tools**

# Architecting a house



**Built most efficiently and timely by a team**

**Requires**


**Modeling**

**Well-defined process**

**Power tools**

# Many stakeholders, many views

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- **many things to many different interested parties**
  - end-user
  - project manager
  - system engineer
  - developer
  - architect
  - maintainer
  - other developers
- **Multidimensional reality**
- **Multiple stakeholders**
  -  multiple views, multiple blueprints

# Lifecycle Phases

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- **Inception** Define the scope of the project and develop business case
- **Elaboration** Plan project, specify features, and baseline the architecture
- **Construction** Build the product
- **Transition** Transition the product to its users

# Architect/Management

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- **Not just a top level designer**
  - **Need to ensure feasibility**
- **Not the project manager**
  - **But “joined at the hip”**
- **Not a technology expert**
  - **Purpose of the system, the “fit”**
- **Not a lone scientist**
  - **Communicator**



# Team Charter

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- **Defining the software architecture**
- **Maintaining integrity of the software**
- **Assessing technical design risks**
- **Proposing the order & contents of iterations**
- **Consultation of stakeholders**
- **Assist in future product definition**
- **Facilitating communications**



# What does the architect need

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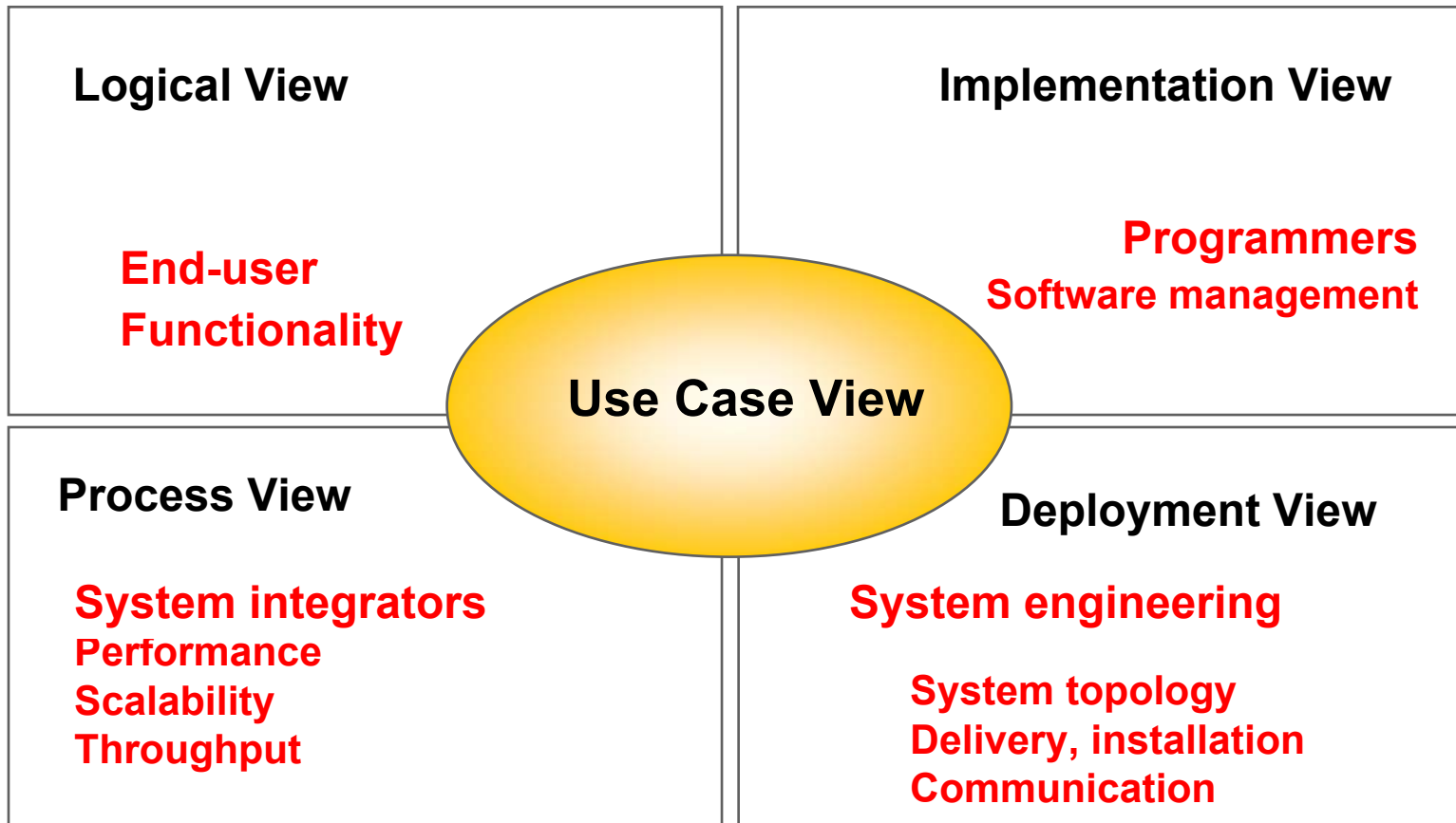
- **Experience**
  - **software development**
  - **domain**
- **Pro-active, goal oriented**
- **Leadership, authority**
- **Architecture team**
  - **balance**

# Models

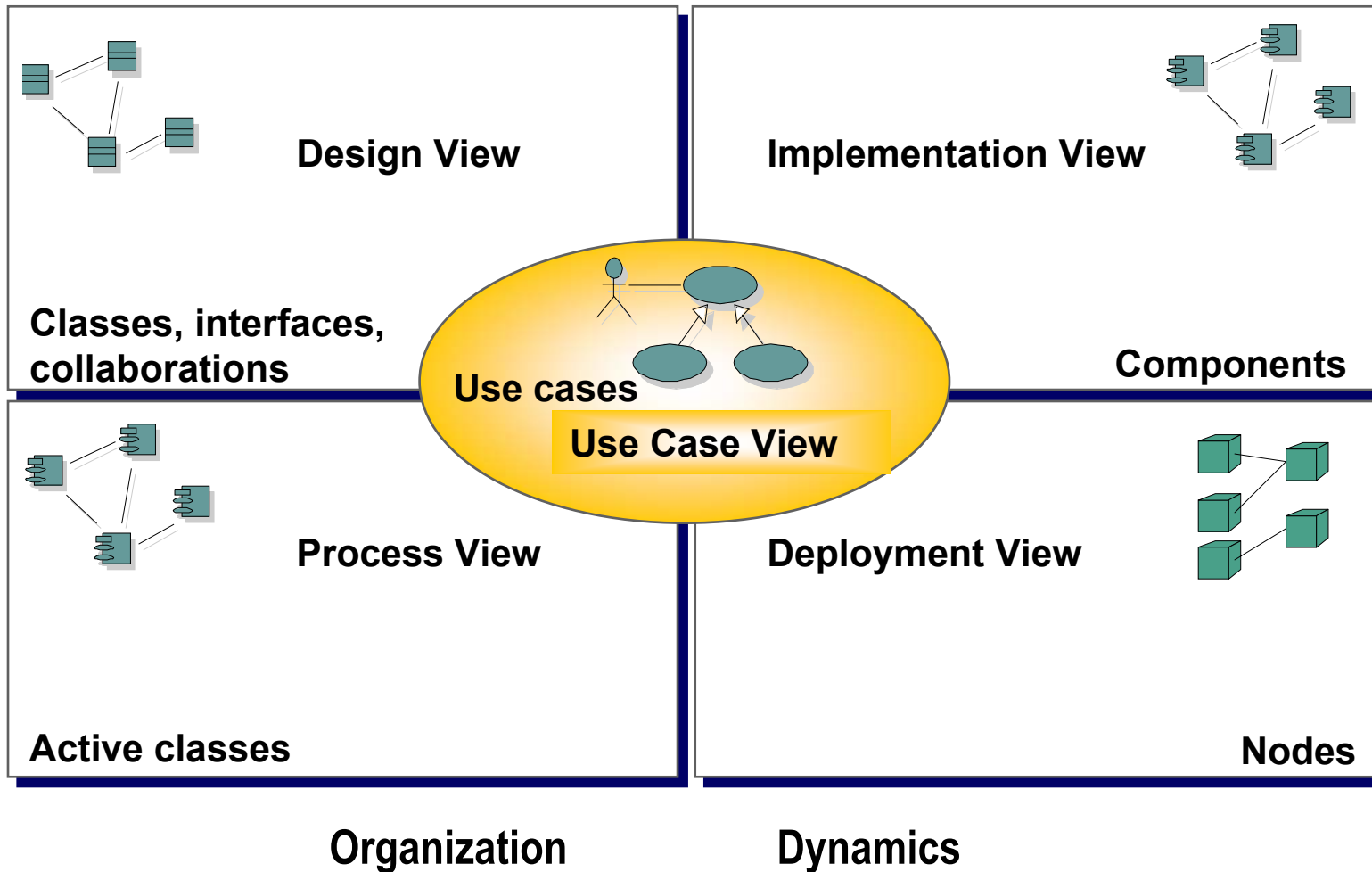
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- **Models are the language of designer, in many disciplines**
- **Models are representations of the system to-be-built or as-built**
- **Models are vehicle for communications with various stakeholders**
- **Visual models, blueprints**
- **Scale**
- **Models allow reasoning about some characteristic of the real system**

# System Architecture



# Architecture and the UML





# The Focus is Interoperability

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- There will *not* be consensus on hardware platforms;
- There will *not* be consensus on operating systems;
- There will *not* be consensus on network protocols;
- There will *not* be consensus on application formats.

**There *must* be a consensus on interoperability.**



# OMG Model Driven Architecture

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An Architectural Style that recommends the use Industry Standard **M**odels, **M**etadata, **M**appings (Patterns & Transformations) for integrating software.

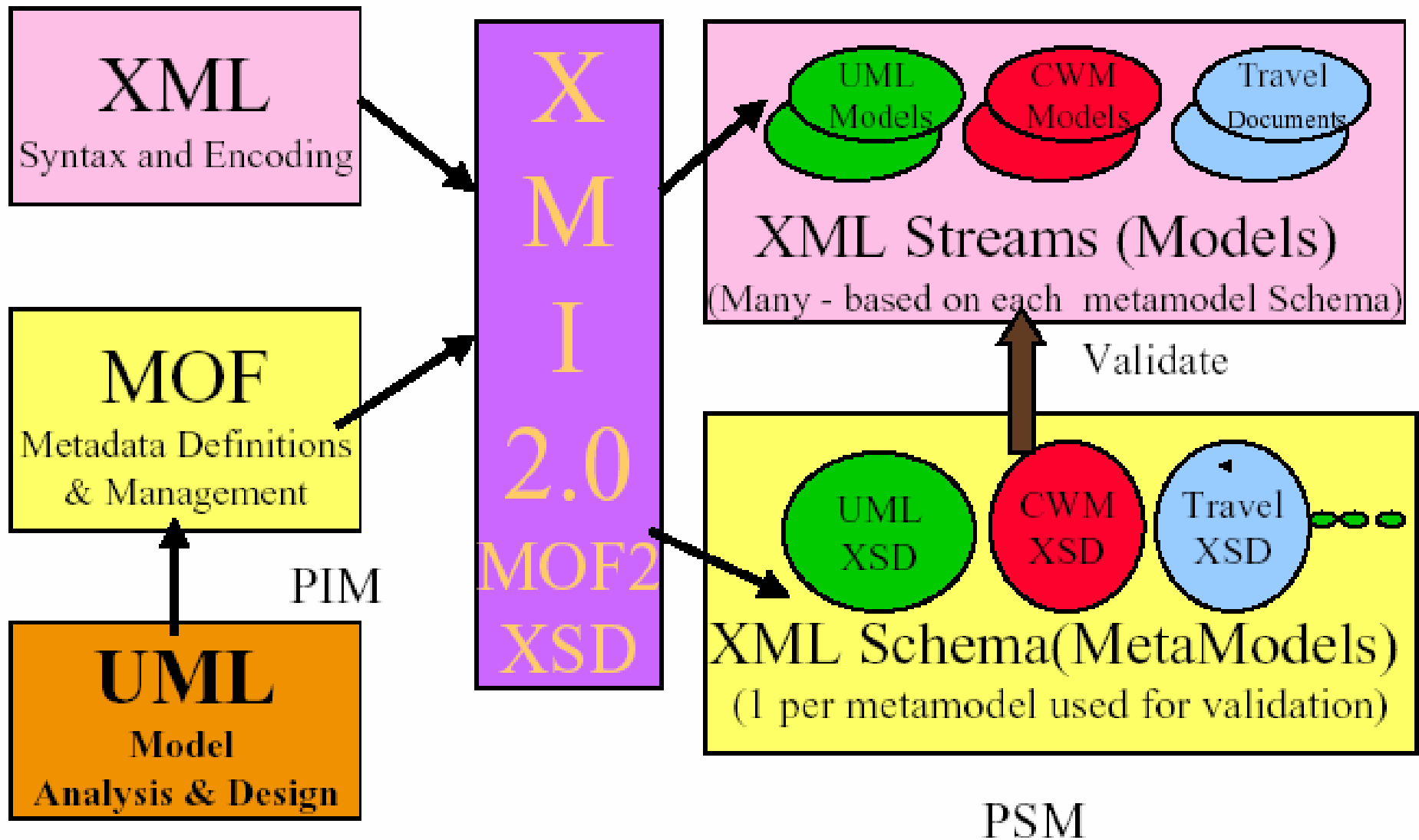
**M**DA allows developers and users to productively *design, build, integrate and manage applications throughout the lifecycle* while separating technology & business concerns.

Sridhar's Usage

# OMG History

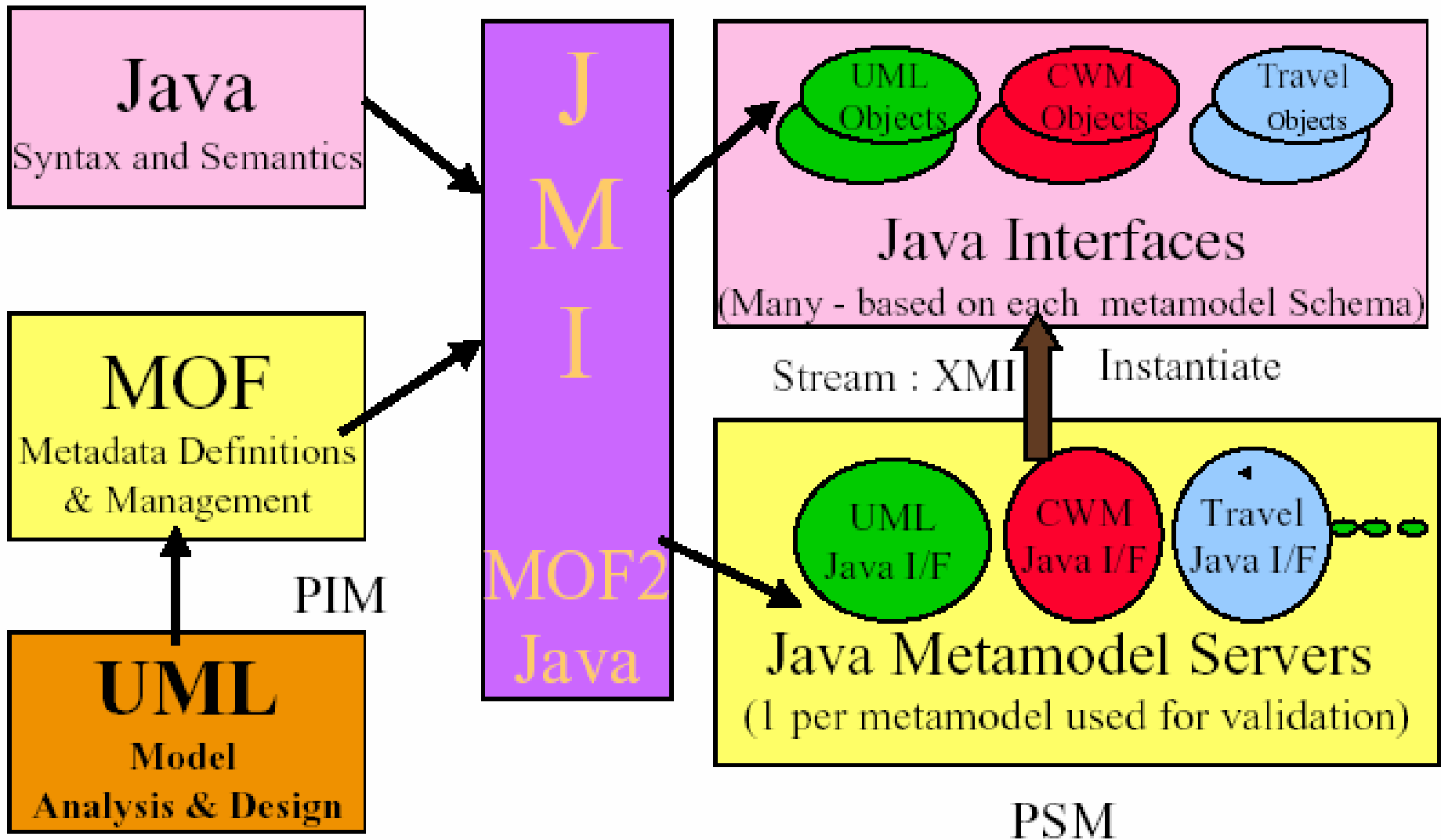
- 700+ Vendors and End User members ([www.omg.org](http://www.omg.org))
- 1989 to 1997 : OMA and CORBA gain prominence
  - 1989 **OMA** Vision & Architecture
  - 1991 **CORBA** 1.0
  - 1995 CORBA 2.0 **IOP** - CORBA Interoperability
- 1995 – 2001 : The foundation for MDA is established
  - 1995 UML and MOF work begins, Java arrives on the scene
  - 1997 **UML** and **MOF** adopted, Domain specs begin to be adopted
  - 1998 XML arrives on the scene, Java and XML gain momentum
  - 1999 **XMI** (integration of MOF, UML and XML) adopted
  - 2000 **CWM**, XMI for XML Schema work begins
  - 2001 UML for EDOC, EAI, UML 2.0 work begins
- 2001 OMG unveils Model Driven Architecture - **MDA**
  - 2002 **XMI 2** adopted, UML2 and MOF 2 proposals arrive
  - 2003 UML2 and MOF2 standards to be adopted
  - 2004 Business Rules and Business Modeling standards expected

# UML\_to\_Schemas (XML) 2002 using XMI





# Models\_to\_Java using JMI 2002





# Middleware Salad Bar

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Capability	J2EE	COM+	CORBA/OMA	Web Services	OMG MDA	.Net
Network Layer	TCP/IP	TCP/IP	TCP/IP	TCP/IP	TCP/IP	TCP/IP
Web Protocol	HTTP	HTTP	HTTP	HTTP	HTTP	HTTP
Interface Definition	Java	Microsoft IDL	CORBA IDL	WSDL	IDL/WSDL...	WSDL/C#
Meta Language	XML	XML	MOF/XML	XML	MOF/XML	XML
RPC Mechanism	RMI/IIOP	DCOM	IIOP	SOAP; XMLP	SOAP; IIOP	SOAP
Registry/Repository	JNDI; LDAP	LDAP; ADSI	CORBA IR	UDDI	MOF;UDDI	UDDI
Process Flow	JPC	Proprietary	Proprietary	BPEL4WS..	UML	BPEL4WS
Modeling Language	UML	UML	UML	UML, XSD?	UML, MOF	UML

**Tiny fragment of the landscape**



# Stages of new technology

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- **“Promise” - this looks good**
- **“Hope” - this seems to work**
- **“Confidence” - this really does work**
- **“Fear” - I might be left behind**
- **“Commitment” - I am in the game now**
- **“Concern” - there seem to be some problems**
- **“Depression” - this isn't easy, and now we are invested**
- **“Perspective” - it has strengths and weaknesses**
  - **we should proceed accordingly**

# UML Diagram Types

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## UML Views

Static View

State Machine View

Activity View

Use Case View

Interaction View

Physical View

Model Mgt View

## UML Diagrams

Class Diagram

Statechart Diagram

Activity Diagram

Use Case (and Diagram)

Sequence Diagram

Collaboration Diagram

Component Diagram

Deployment Diagram

Package Diagram

## Visual Editor Project

First-class GUI building tools for Eclipse

[www.eclipse.org/vep](http://www.eclipse.org/vep)



### Eclipse Visual Editor Project

The Eclipse Visual Editor project is a framework for creating GUI builders for Eclipse. It will include reference implementations of Swing/JFC and SWT GUI builders, but intends to be useful for creating GUI builders for other languages such as C/C++ and alternate widget sets, including those that are not supported under Java.

## UML2

EMF-based UML 2.0 Metamodel Implementation

[www.eclipse.org/uml2](http://www.eclipse.org/uml2)

### UML2 Project

UML2 is an EMF-based implementation of the UML 2.0 metamodel for the Eclipse platform. [more...](#)

## GMT

Generative Model Transformer



<http://www.eclipse.org/gmt/>

### Welcome

The goal of the Generative Model Transformer project is to construct/assemble a set of tools for model driven software development with fully customisable Platform Independent Models, Platform Description Models, Texture Mappings, and Refinement Transformations.

*Workflow Management Coalition*

**WfM**  
**fC**

**Workflow**

**XPDL**

*The Workflow Management Coalition Specification*

Workflow Management Coalition  
Workflow Standard

Workflow Process Definition Interface  
-- XML Process Definition Language



# What is Workflow

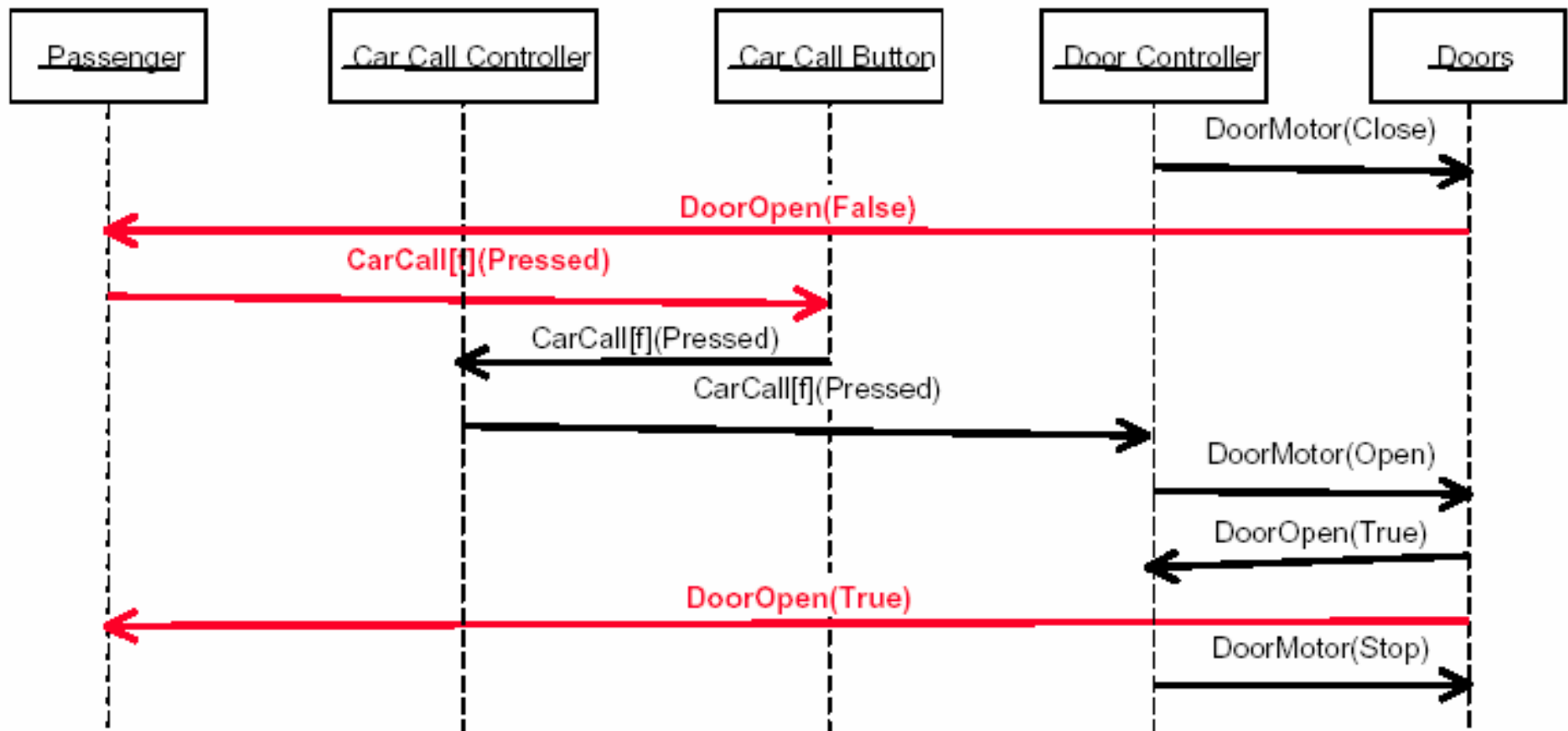
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**A characteristic of an environment that can benefit from workflow, is the presence of many different tasks and activities, where information must be passed between these according to a predefined set of rules.**

**From the *WfMC*, the Workflow Management Coalition**

# Sequence Diagram

Constructing sequence diagram should just be a matter of connecting messages from your scenario in the right order:





# JAWE Java Workflow Editor

Process properties - EOrder

Applications | Workflow relevant data | Formal parameters | Redefinable header | Participants

General | Process header

Id: 1  
Name: EOrder

CreditCheck

Process properties - EOrder

General | Process header | Redefinable header | Participants

Applications | Workflow relevant data | Formal parameters | Activities | Transitions | Activity sets

Formal parameters

Id	Index	Mode	Data type
orderString	1	In	Basic type - String
returnMessage	2	Out	Basic type - String

New Edit

Process properties - EOrder

General | Process header | Redefinable header

Applications | Workflow relevant data | Formal parameters | Activities | Transitions

Activities

Id	Name	Performer
1	Check Data	
5		
6		
8	Email Confirmation	
9		
10	Check Credit Subprocess	
11	Fill Order Subprocess	
12	Check Order Type	
17	Transform Data	
32	Enter Order	DBConnection - sys
33		
39	Compose RejectionMessage	
41	Check Vendor Account	DBConnection - sys
56	Compose Acceptance Message	
58	Raise Alarm	

New Edit Delete

One or more processes have log

Graph view | XPDL view



## Bronstee.com

### Software & Services

*the source site*

tools for uml modeling and java(tm) application development. consultancy in java and component based technologies.

[info@bronstee.com](mailto:info@bronstee.com)

Bronstee.com is a small company, specializing in **generative, model driven** java application development tools and in services related to java application development.

[Read more...](#)

A group of people have started a website for information on **model-driven software development**: <http://www.mdsd.info>. Take a look... this website is sponsored by bronstee.com.

### **FUUT-je**

The Fantastic, Unique, UML Tool for the Java Environment.

FUUT-je is a tool to create prototypes of Java applications. It uses a simplified UML modeling environment, and it generates Java source code from your model. Read more at Services....

[Read more...](#)

**Generative Model Transformer**, an Open Source project at [www.eclipse.org](http://www.eclipse.org).

[Read more here...](#) or, link directly to: [Eclipse](#).

# Techniques to Implement Workflow

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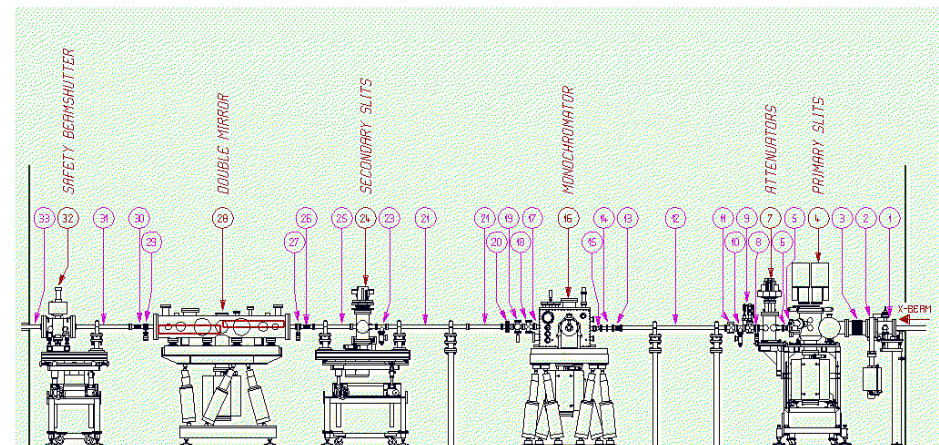
- Starting point is XPD, as modeled in an XML Schema.
- Use FUUT-je, a text/code generation component for GMT, to transform the schema to a UML class diagram.
- Generate Java code from the UML model.
- Develop a UML class diagram for the Workflow Enactment service.
- Generate Java code from the UML model using FUUT-je.



# What is all this to do with

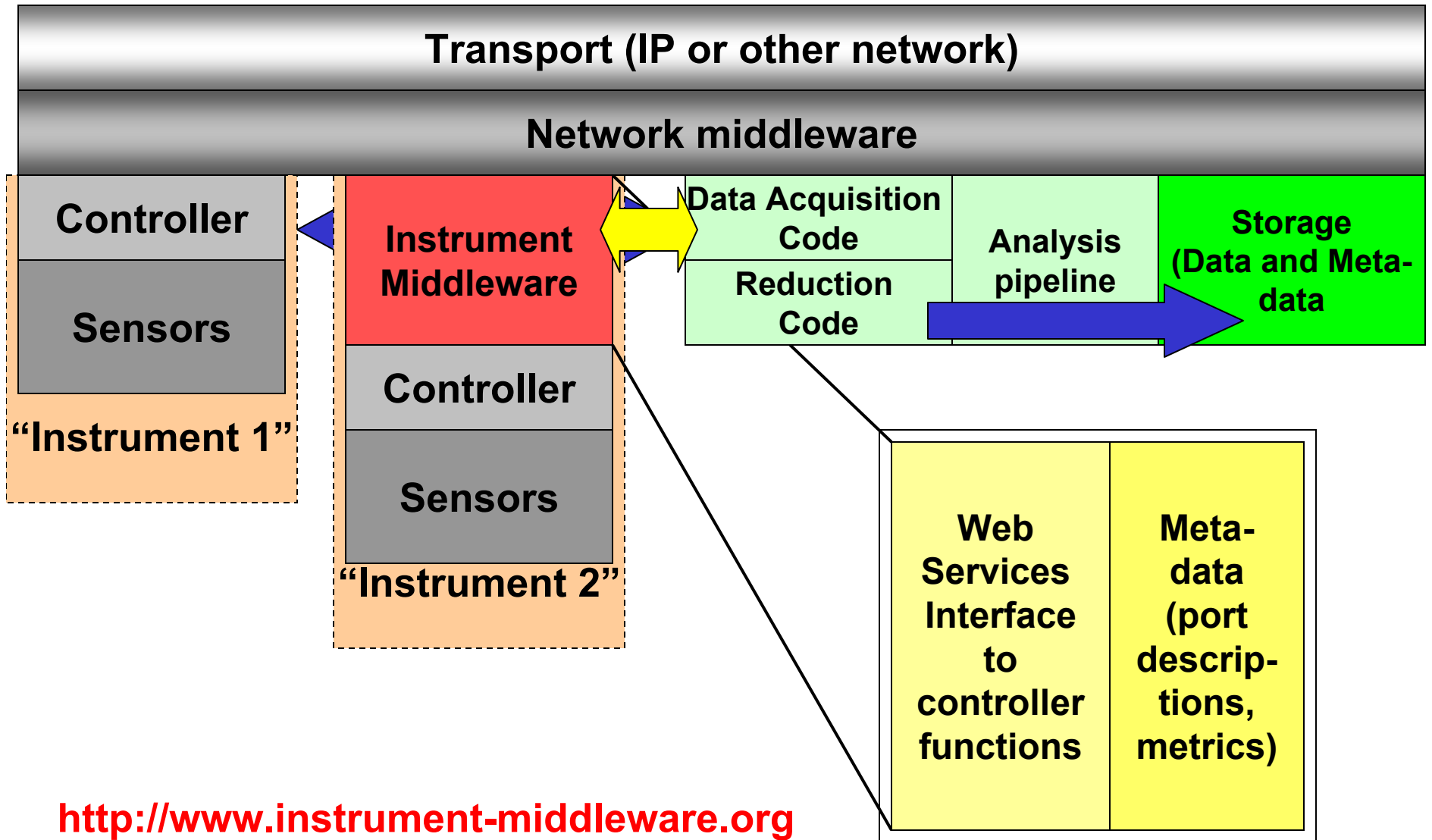
- equipment timing
- beam steering
- slit drives
- beamline monochromators
- endstation instrumentation
- movable photon masks
- Temperature monitoring
- radiation monitoring
- beam shutters.

## Instrument Management

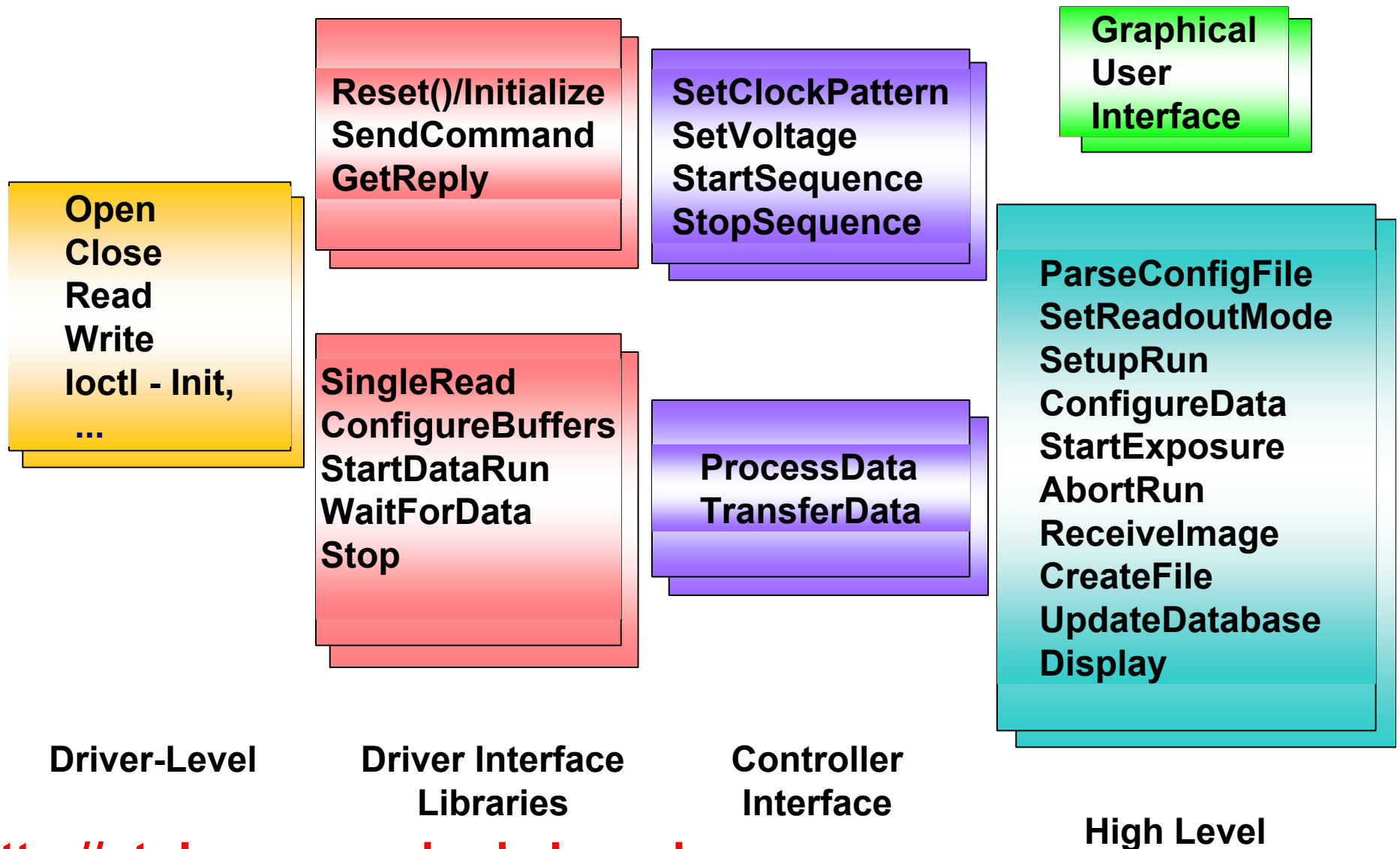


1003 - LINE AND OPTICS COMPONENTS IN OPTICS HUTCH

# Common Instrument Middleware



# Ptolemy Project and Actor-Oriented Design



Finally, remember:

**People...**

Not Tools

Not Techniques

Not Methodologies

**...Build Applications**









# Beam line Definition



# DESY Beamlines in the PDB

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DESY X11	'DESY HAMBURG'	DESY X11	'DESY, HAMBURG'
DESY X11	'DESY, HAMBURG;'	DESY X11	'DESY,HAMBURG'
DESY X11	'DESY-EMBL HAMBURG'	DESY X11	'DESY-EMBL,HAMBUR'
DESY X11	'DESY-EMBL,HAMBURG'	DESY X11	'DESY-EMBL,HAMBURG BEAMLINE X11'
DESY X11	'DESY/EMBL, HAMBURG'	DESY X11	'DESY; HAMBURG;'
DESY X11	'EMBL-DESY, HAMBURG'	DESY X11	'EMBL/DESY HAMBURG, BEAMLINE X11'
DESY X11	'EMBL/DESY, '	DESY X11	'EMBL/DESY, HAMBU'
DESY X11	'EMBL/DESY, HAMBU -GBF/'	DESY X11	'EMBL/DESY, HAMBURB'
DESY X11	'EMBL/DESY, HAMBURG'	DESY X11	'EMBL/DESY, HAMBURG ;'
DESY X11	'EMBL/DESY, HAMBURG ; MPG'	DESY X11	'EMBL/DESY, HAMBURG BEAMLINE X11'
DESY X11	'EMBL/DESY,HAMBURG'	DESY X11	'EMBL/DESY,HAMBURG BEAMLINE X11'
DESY X11	'HASYLAB, HAMBURG'	DESY X11	'EMBL/DESY,HAMBURG BEAMLINE X11, '
DESY X11	'MPG/DESY'	DESY X11	'MPG/DESY HAMBURG'
DESY X11	'MPG/DESY, HAMBURG'	DESY X11	'MPI/DESY HAMBURG'
DESY X11	'MPI/DESY, HAMBURG'	DESY X31	'DESY-EMBL,HAMBURG BEAMLINE X31'
DESY BW6	'DESY, HAMBURG BW6'	DESY X31	'EMBL/DESY, HAMBURG BEAMLINE X31'
DESY BW6	'DESY/HAMBURG, BW6'	DESY BW6	'EMBL/DESY, HAMBURG BEAMLINE BW6'
DESY BW7A	'DESY-EMBL,HAMBURG BEAMLINE BW7'	DESY BW7A	'EMBL/DESY, HAMBURG BEAMLINE BW7A'
DESY BW7A	'EMBL/DESY,HAMBURG BEAMLINE BW7A'	DESY BW7B	'EMBL/DESY, HAMBURG BEAMLINE BW7-B'
DESY BW7B	'EMBL/DESY, HAMBURG BEAMLINE BW7B'	DESY BW7B	'DESY-EMBL,HAMBURG BEAMLINE BW7B'
DESY BW7B	'EMBL/DESY,HAMBURG BEAMLINE BW7B'	DESY JENA	'IMB JENA/U.HAMBURG/EMBL/DESY, '



## Beam line Definition

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<code>_sync_beam_light_source.sync_id</code>	<b>ESRF</b>
<code>_sync_beam_light_source.beam_line_id</code>	<b>BM14</b>
<code>_sync_beam_light_source.type</code>	<b>'Bending magnet (BL02B1)'</b>
<code>_sync_beam_light_source.Critical_energy</code>	<b>28.9 keV</b>
<code>_sync_beam_light_source.Source_size_sx</code>	<b>0.182 mm</b>
<code>_sync_beam_light_source.Source_size_sy</code>	<b>0.058 mm</b>
<code>_sync_beam_light_source.Source_size_sy_prime</code>	<b>'0.065 mrad(@10 keV)'</b>
<code>_sync_beam_light_source.Horizontal_beam</code>	<b>'1.5 mrad divergence'</b>
<code>_sync_beam_light_source.type</code>	<b>'In-vacuum undulator'</b>
<code>_sync_beam_light_source.Undulator_period</code>	<b>32 mm</b>
<code>_sync_beam_light_source.Number_periods</code>	<b>140</b>
<code>_sync_beam_light_source.Tunable_range</code>	<b>'&gt; 9 keV'</b>
<code>_sync_beam_light_source.Peak_brilliance</code>	<b>'2x10<sup>19</sup>photons/s/mrad<sup>2</sup>/mm<sup>2</sup>/0.1%b.w.(I=100mA)'</b>
<code>_sync_beam_light_source.Total_power</code>	<b>5 kw</b>
<code>_sync_beam_light_source.Power_density</code>	<b>'300 kW/mrad<sup>2</sup>'</b>