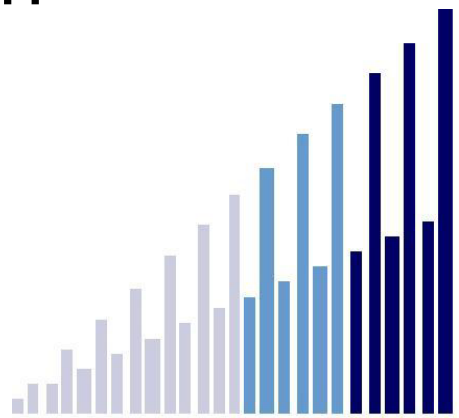
Integrating High Throughput Workflows: Value and Build vs. Buy Analyses (Plus A Bit More)

ACS Fall Meeting

CINF Emerging Trends in Discovery Data Integration

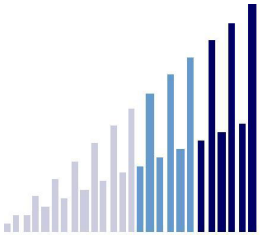
Peter E. Cohan
The Second Derivative

September 10, 2003

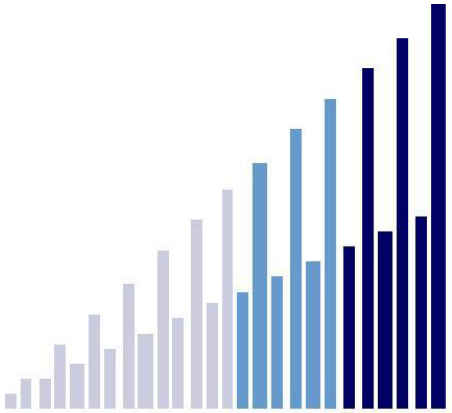


Agenda

- Some Definitions of “Integration”
- Workflow Value Analysis
- Workflow Software Build vs. Buy Analysis
- Impact of Demonstrations and Ideas to Improve Results
- Summary



Some Definitions of “Integration”



Definitions of “Integration”

1. Customer’s Perspective:

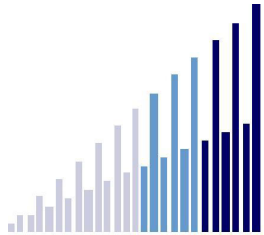
   Data or information that we need to bring together to solve a problem we face today.

2. Vendor’s Perspective:

   Data or information that we can bring together to solve a problem we hope our customers face today.

3. Visionary’s Perspective:

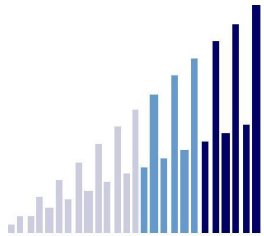
   Data or information that it would be really cool to bring together to enable some really cool things…



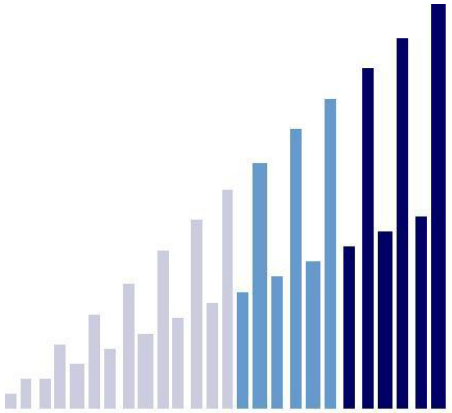
Definitions of “Integration”

Workflow Perspective:

- “Integration” is the enabling of a workflow and its results from the perspective of a workflow user or beneficiary.
- A “workflow” can include 1 or more linked, nested, or concurrent other workflows
  - (e.g. the drug discovery and development pipeline)
- A workflow can include hardware, software, and know-how
  - The definition of a workflow is in the eye of the beholder…

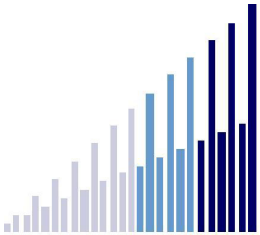


High Throughput Workflows – Value Analysis



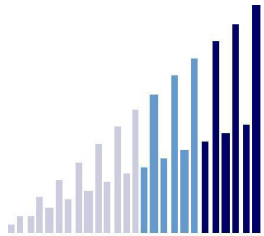
Pre-Summary

- If you know what you want to accomplish, and the problem is tractable, then high-throughput methods pay-off big time…



Where Can We Apply High Throughput Methods?

- Pharma Discovery
  - Combinatorial and Parallel Synthesis
  - Synthetic Methods Scoping and Development
  - High Throughput Screening
  - Toxicology, ADME
- Pharma Chemical Development
  - Process Development
  - Polymorphs and Salt Selection
  - Formulation
- Materials Science
  - Homogeneous Catalysis (e.g. Polyolefins)
  - Heterogeneous Catalysis
  - Pigments
  - Polymers, Coatings and Formulations
  - Electronic Materials (e.g. Phosphors, Fuel-Cells)



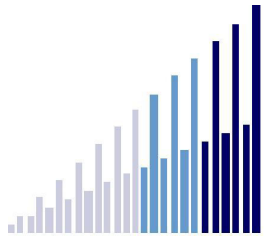
Key Business Objectives

There needs to be an economic driving force:

- Dramatically increase the rate of innovation in the discovery and optimization of…
- Implement high throughput core competency…
- Achieve cultural change from traditional to high throughput methods…

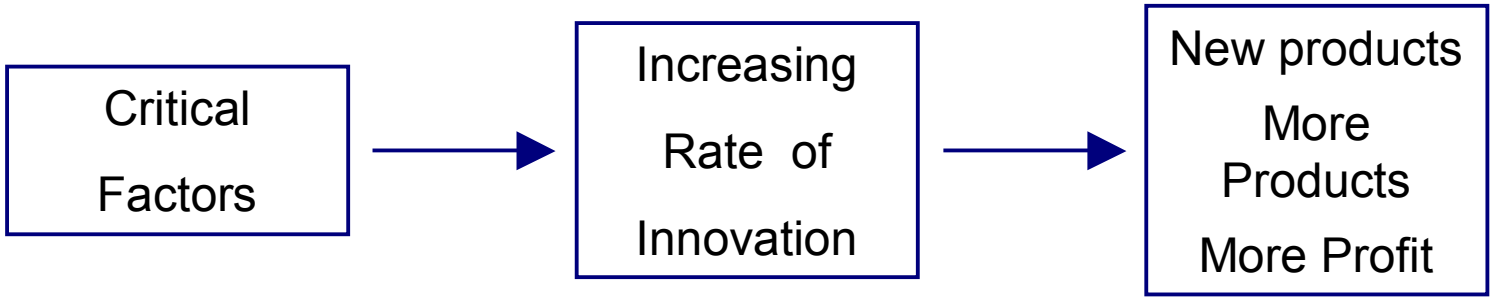
For Example:

- "We need a critical commercializable discovery in a key business area"
- "We just had a critical commercializable discovery in a key business area
  - And we need to exploit and protect it rapidly"



Workflow Value Analysis

- Understand the value chain
- Identify the critical, measurable values
- Estimate the value of high throughput research and/or optimization



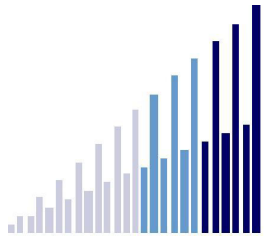
Critical Factors

- Improve the probability of success of projects
- Perform more projects with the same resources
- Reduce the time to market

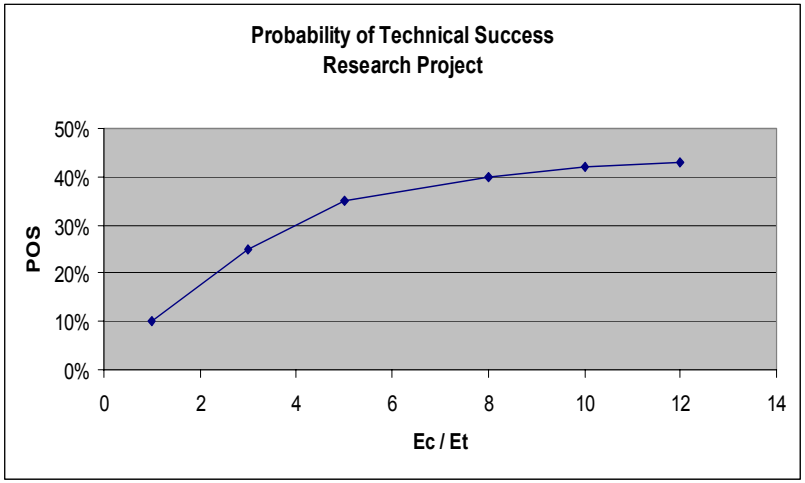
Measurable

- Make critical business/market decisions earlier
- Increase visibility into projects' success or failure ("fail early")
- Present the best candidate to the next phase
- Improve IP protection and management of competitive IP
- Capitalize rapidly on opportunities
- Uncover unexpected results and discoveries

Valuable, but Intangible

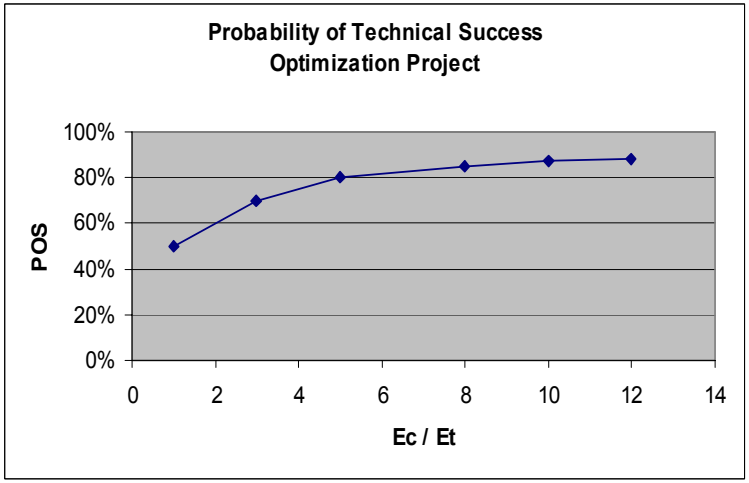


Measurable Value: Increase Probability of Success



Long-term Research Projects

Optimization Projects



Data Sources:

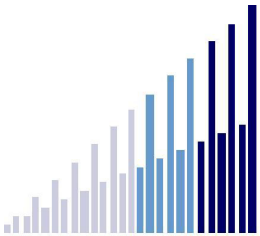
- Dow, ExxonMobil, W.R. Grace, Symyx Technologies

Types of R&D Projects

	"Research"	"Optimization"	"Firefighting"
% of R&D Work	17%	57%	26%
FTE Rate / Pair (1 Pair = 1 Scientist + 1 Technician)	$560K / year	$560K / year	$560K / year
Experiments per Year (per Pair)	435	610	610

Data Sources:

- Dow, ExxonMobil, W.R. Grace, Symyx Technologies



Throughput Assumptions

- Workflow includes:
  - Specification
  - Synthesis
  - Sample Preparation
  - Screening
  - Data Management and Analysis
- All steps are equally matched in throughput with one another
  - [**No bottlenecks**]
- Each "Cell" can be run once per day (200 working days per year) - **sustainable**
  - 24 cells = 4,800 experiments per year
  - 48 cells = 9,600 experiments per year
  - 96 cells = 19,200 experiments per year
- Metrics:

	"Research"	"Optimization"	"Firefighting"
% of R&D Work	17%	57%	26%
FTE Rate / Pair (1 Pair = 1 Scientist + 1 Technician)	$560K / year	$560K / year	$560K / year
Experiments per Year (per Pair)	435	610	610

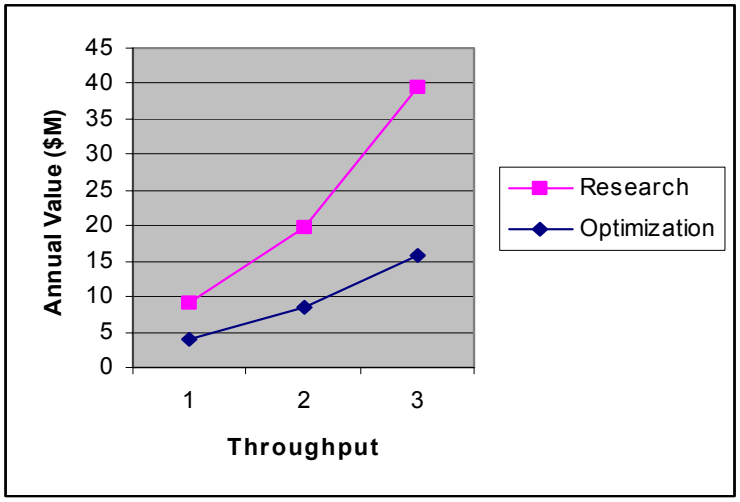
Value Calculation Examples

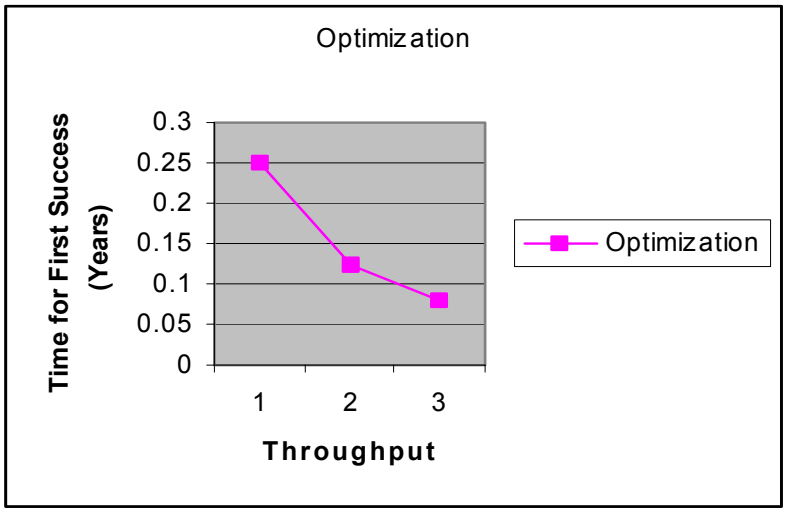
- Case I: Optimization
  - Ia: 24 cell system used by a team of 1 pair (2 people)
  - Ib: 48 cell system used by a team of 1 pair (2 people)
  - Ic: 96 cell system used by a team of 2 pairs (4 people)
  - Id: 48 cell system used by a team of 1 pair (2 people) with increased POS
- Case II: Research
  - IIa: 24 cell system used by a team of 2 pairs (4 people)
  - IIb: 48 cell system used by a team of 2 pairs (4 people)
  - IIc: 96 cell system used by a team of 2 pairs (4 people)
  - IId: 48 cell system used by a team of 2 pairs (4 people) with increased POS
- Case III: Combined Research and Optimization
  - IIIa: 96 cell system used by a team of 2 pairs (4 people) – 1 research success
  - IIIb: 96 cell system used by a team of 2 pairs (4 people) – 2 research successes

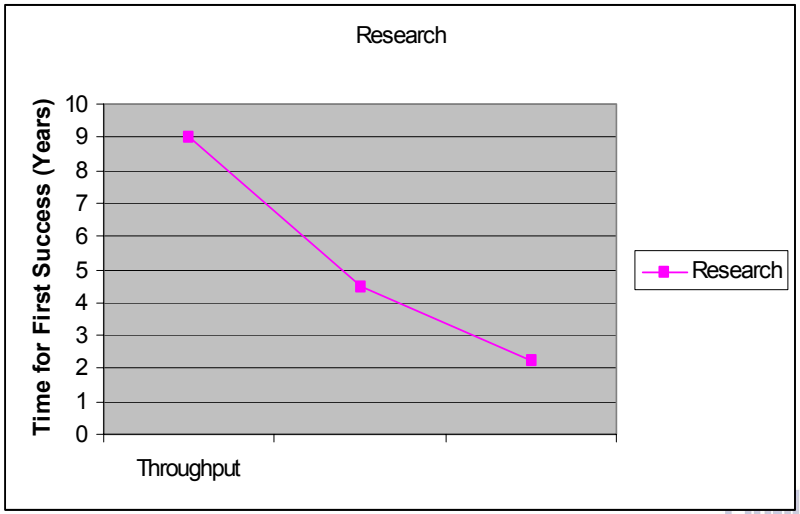
Summary – Comparison of Traditional vs. High Throughput

Case	Traditional Time to First Success	HT Time to First Success	Annual Value of HT System
Optimization 24	2 years	3 months	$3.9M
Optimization 48	2 years	1.5 months	$8.4M
Opt. 96 (2 pairs)	2 years	0.8 months	$15.7M
Opt. 48 ↑ POS	2 years	4 months	$2.1M
Research 24	50 years	9 years	$5.1M
Research 48	50 years	4.5 years	$11.3M
Research 96	50 years	2.25 years	$23.8M
Res. 96 ↑ POS	50 years	2.82 years	$18.7M
Combined 1	50/2 years	2.25yr/0.8 month	$19.3M
Combined 2	50/2 years	2.25yr/0.8 month	$19.3M

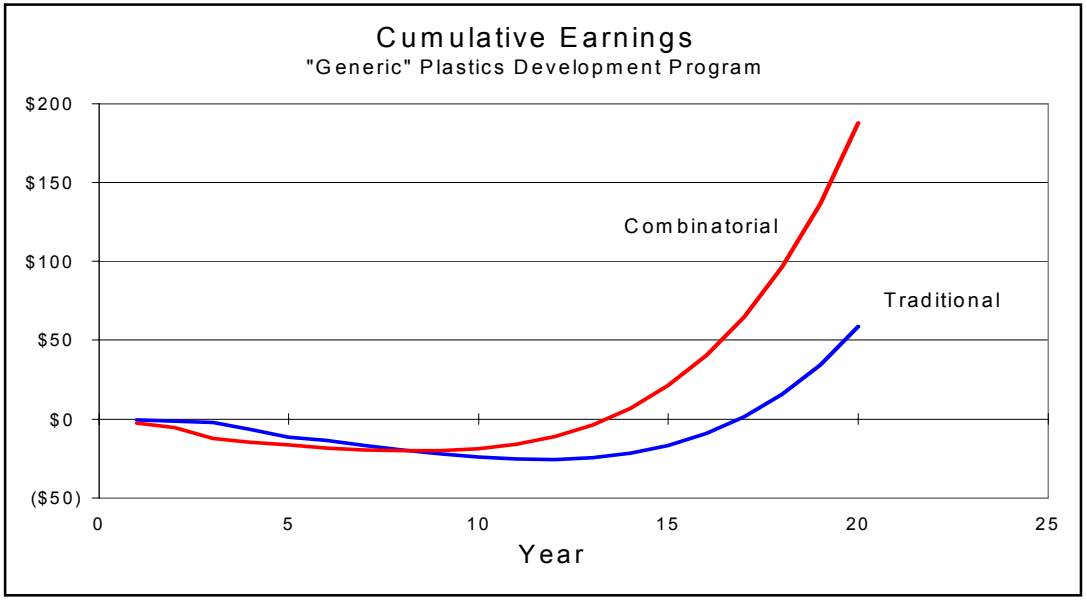
Summary – Sensitivity Analysis





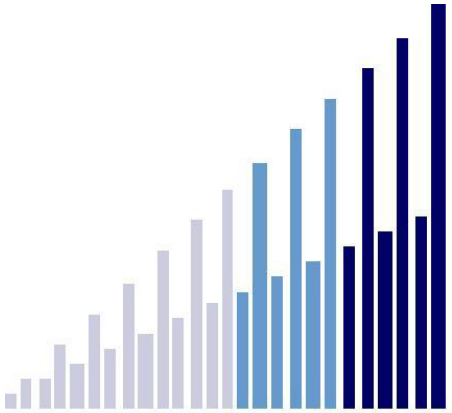


Summary – Cost per Experiment and Pro-Forma Analysis



	Cost Per Experiment Over 3 Years	Cost Per Experiment Over 5 Years
Industry Today	$1075	$1075
Commercial System at 12,000 Experiments / Year	194	97
Commercial System at 24,000 Experiments / Year	135	68

Workflow Software Build vs. Buy Analysis



Pre-Summary: "Core" or "Context"?

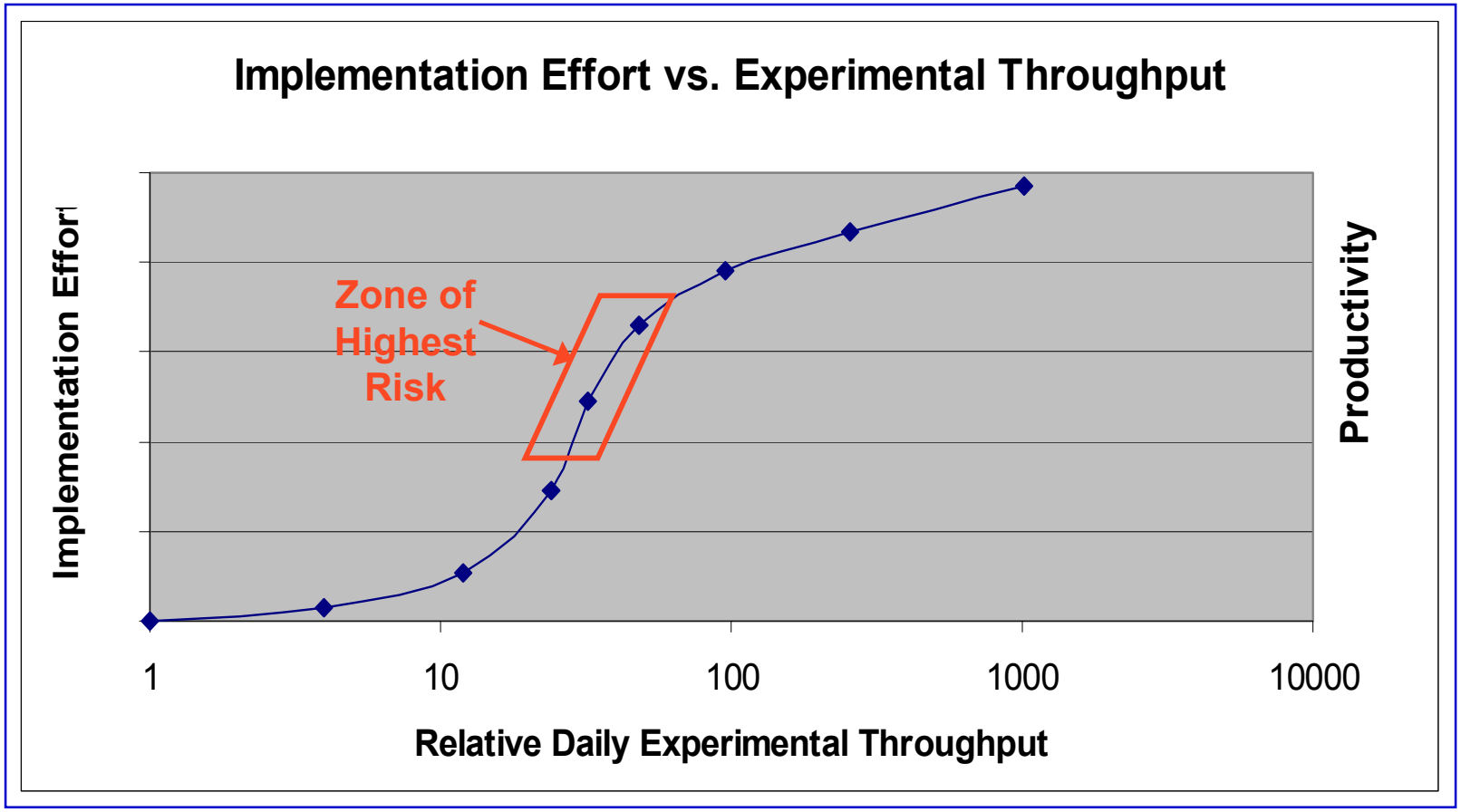
- Core: Stuff that makes your business what it is
- Context: Stuff that has to be done but does not really differentiate

- Recommendation:

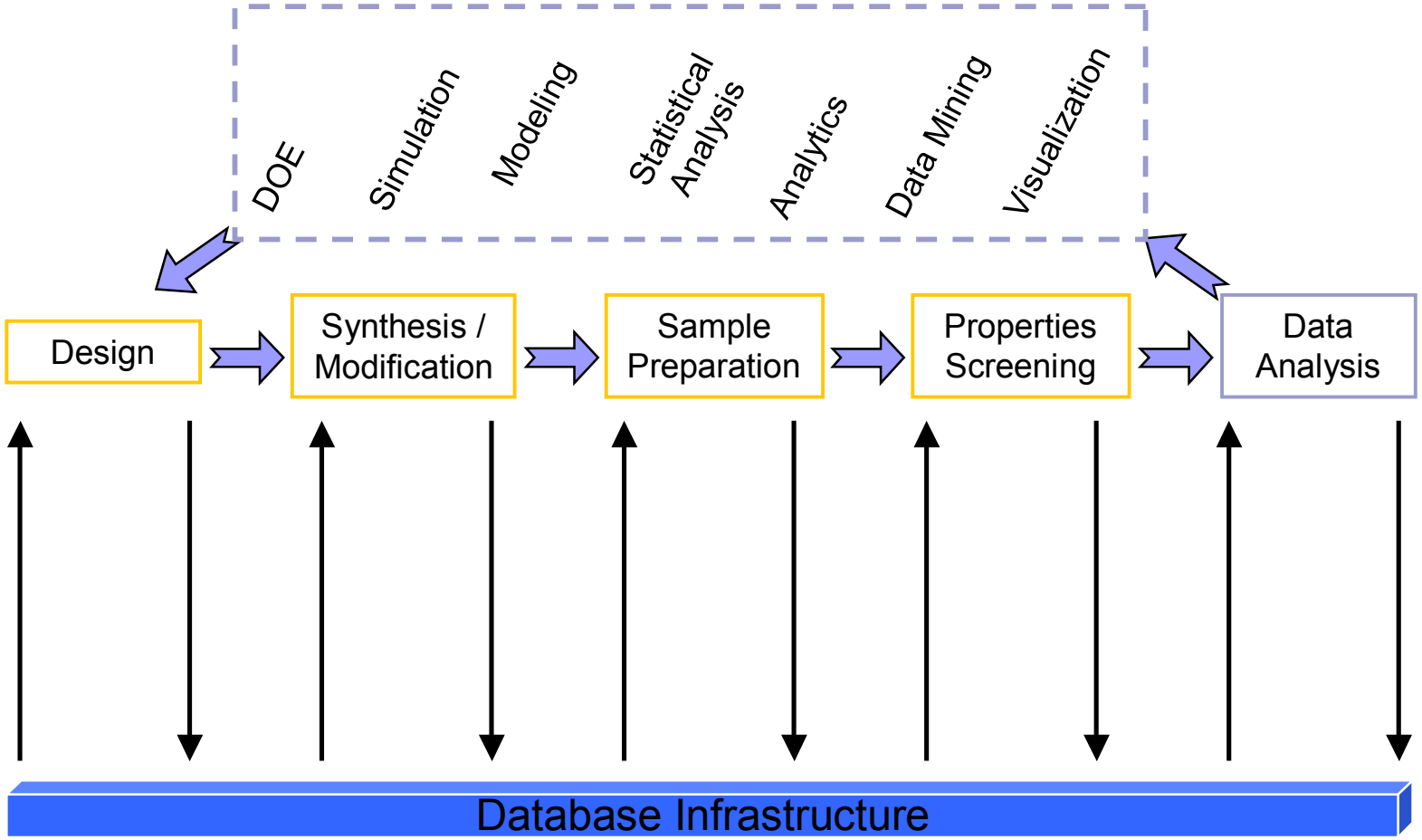
  Invest in "Core", Outsource "Context"

  - Geoffrey Moore

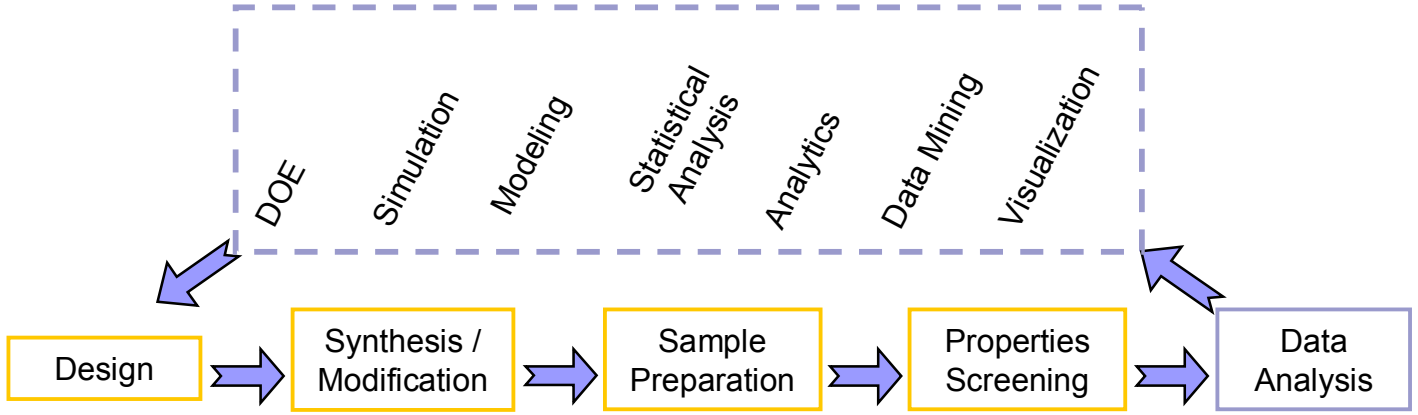
Implementation Effort vs. Productivity



Workflow and Implementation Requirements

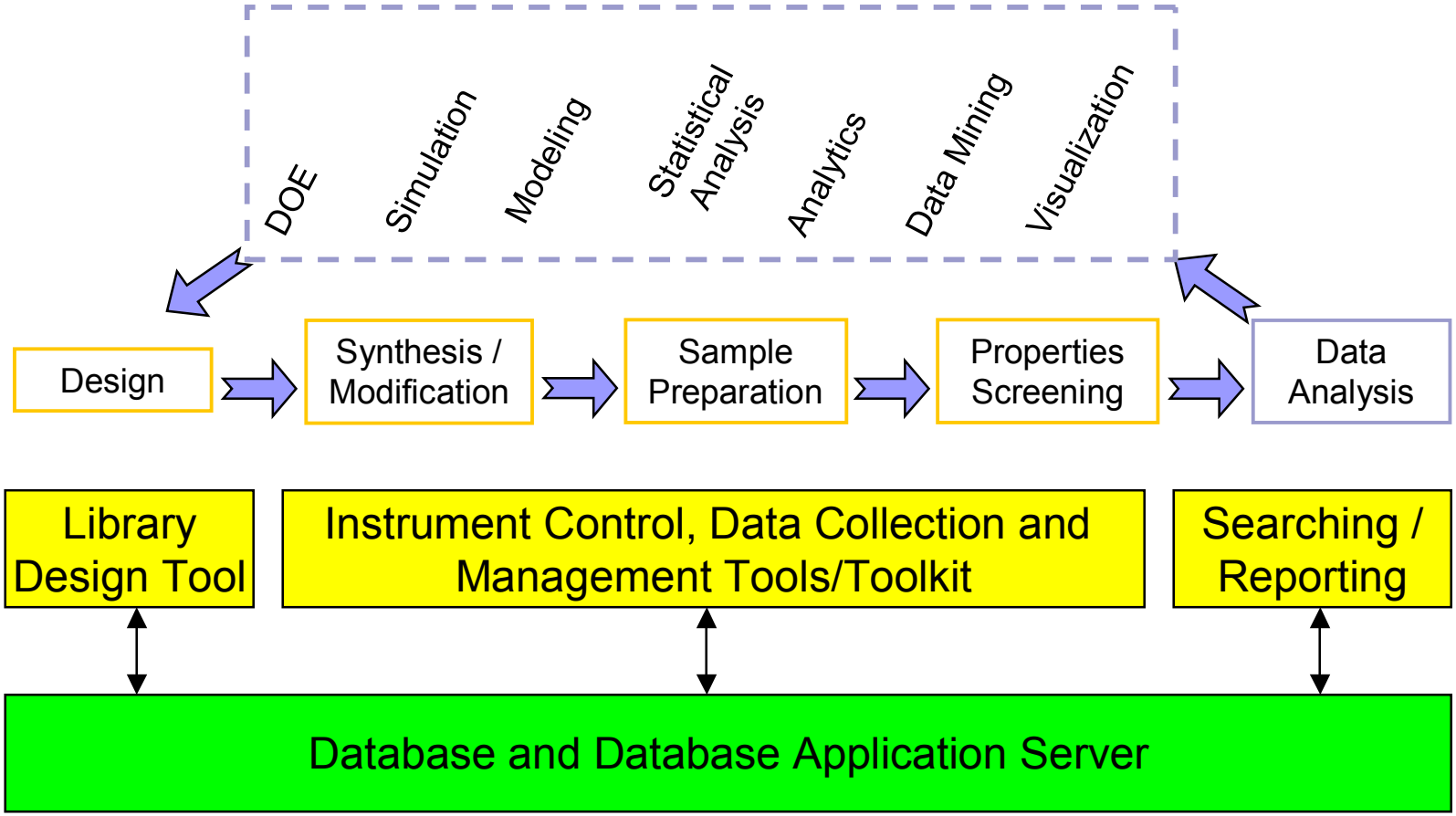


Workflow and Implementation Requirements

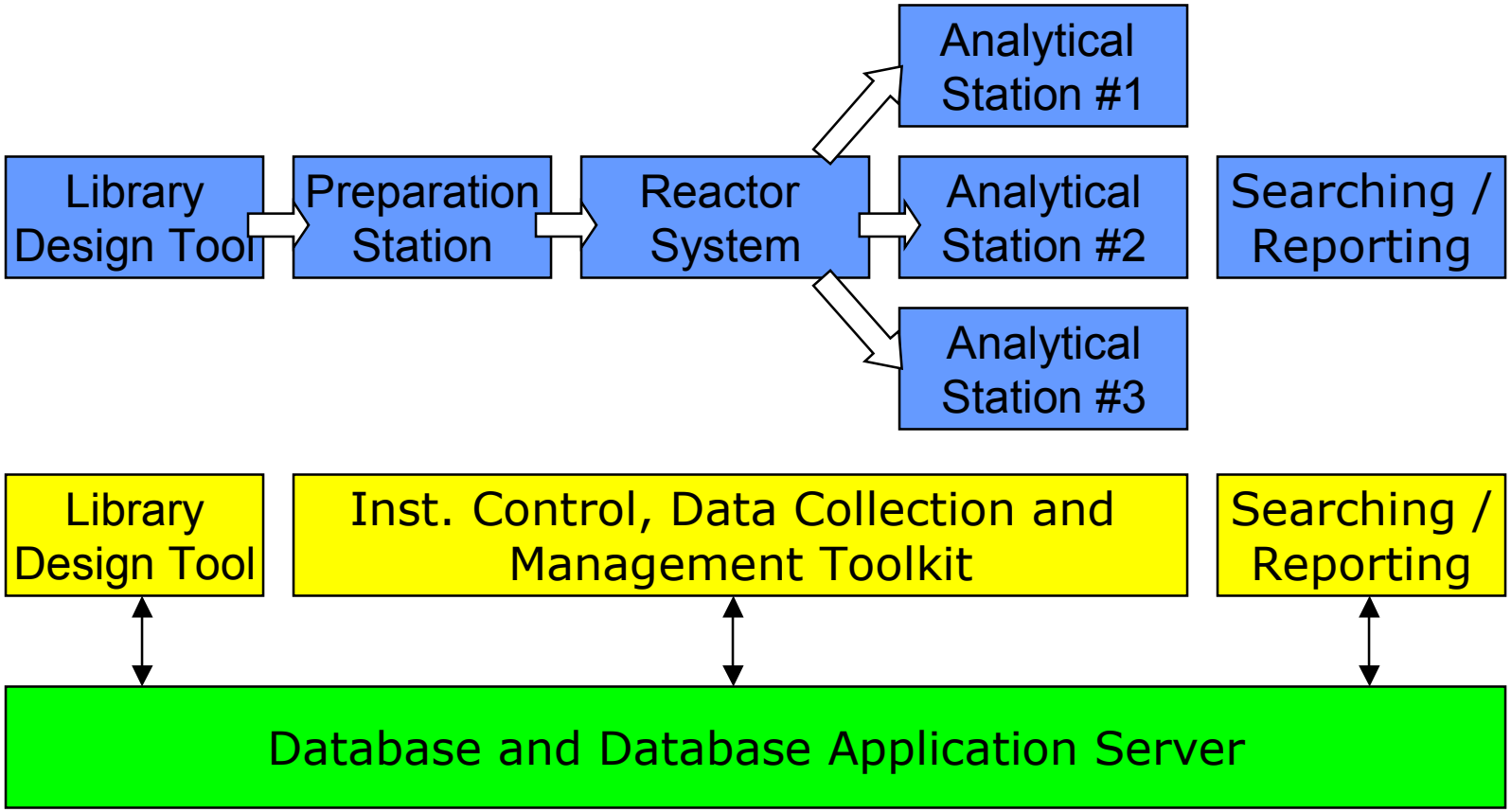


Hardware	N/A	✓	✓	✓	N/A
Instrument Control SW	N/A	✓	✓	✓	N/A
End User SW	✓	✓	✓	✓	✓
Data Collection / Workflow Mgt. SW	N/A	✓	✓	✓	✓
Database	✓	✓	✓	✓	✓
Know-How	✓	✓	✓	✓	✓

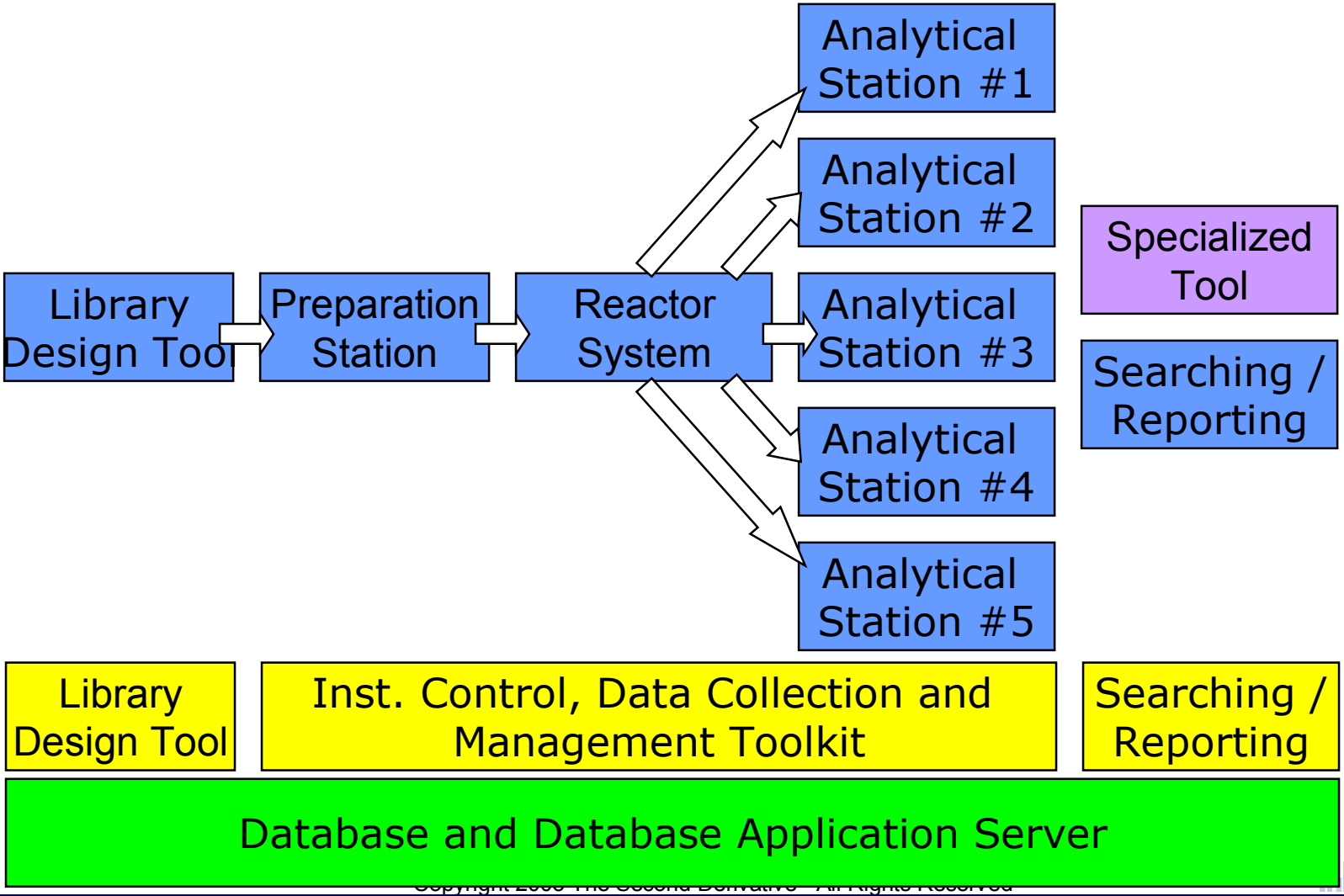
Generalized Informatics Blocks Implemented at Example Company



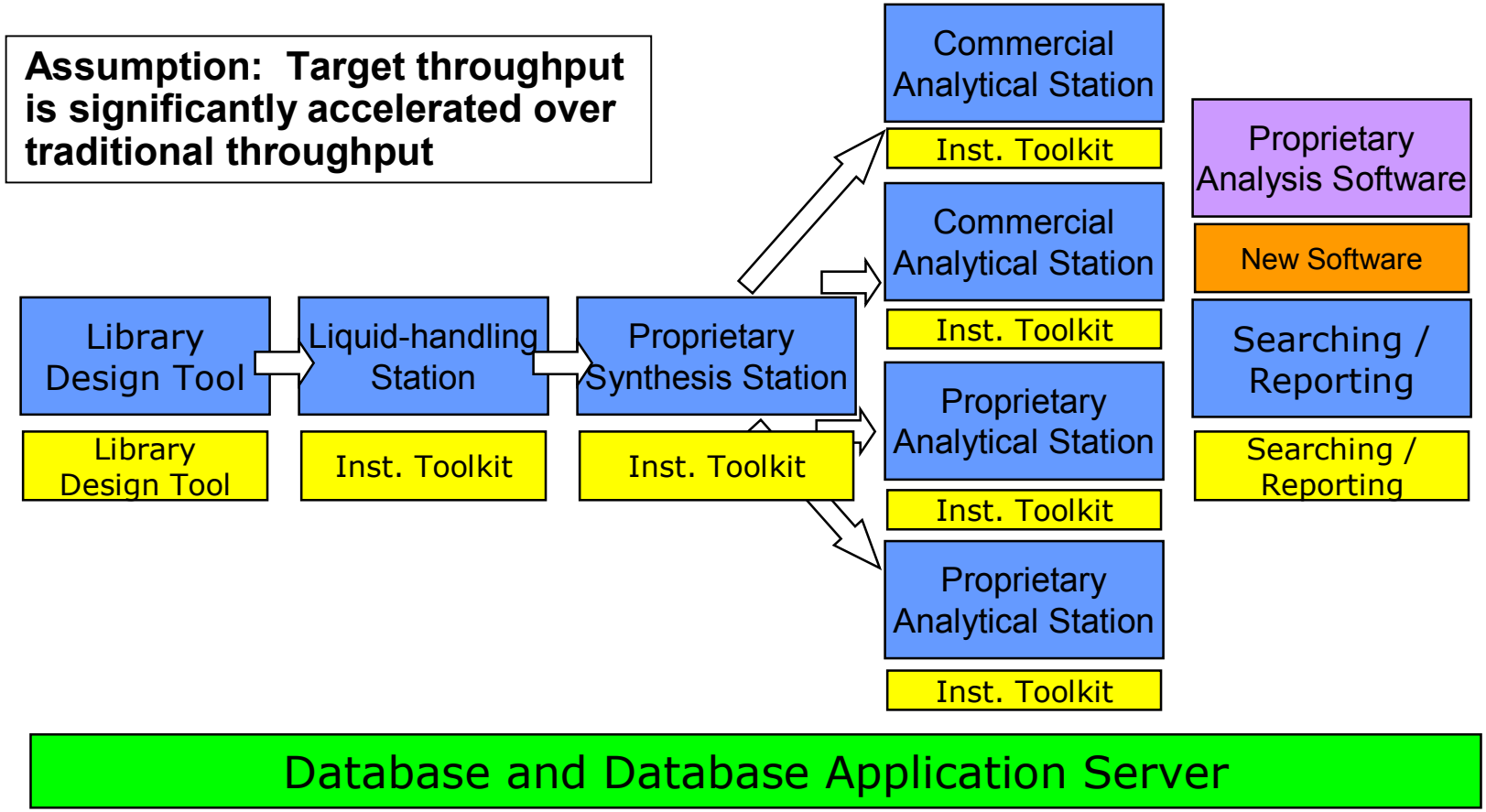
First Workflow – Informatics Blocks



Second Workflow – Informatics Blocks



New Workflow at Example Company– Module Blocks



New Workflow – Informatics Implementation Based on Existing Foundation

Software Implementation Effort at Company (based on Existing Foundation):

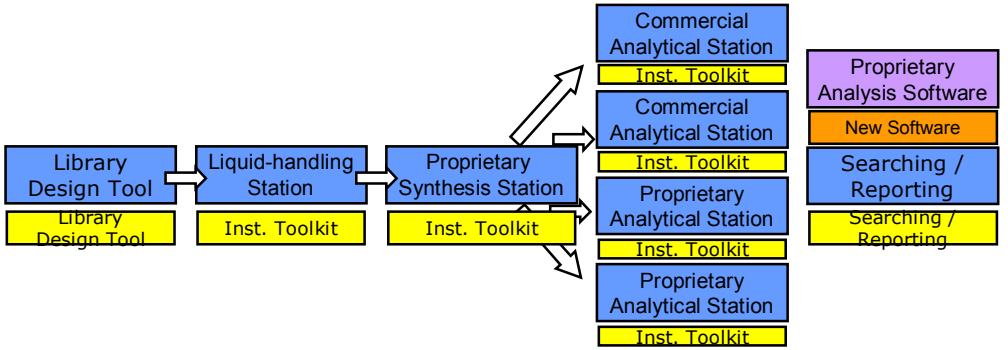
67 months (~5.5 person-years), over a period of 16 months

Staffing and Disciplines (SW Only):

9 individual staff members, in addition to the core foundation team

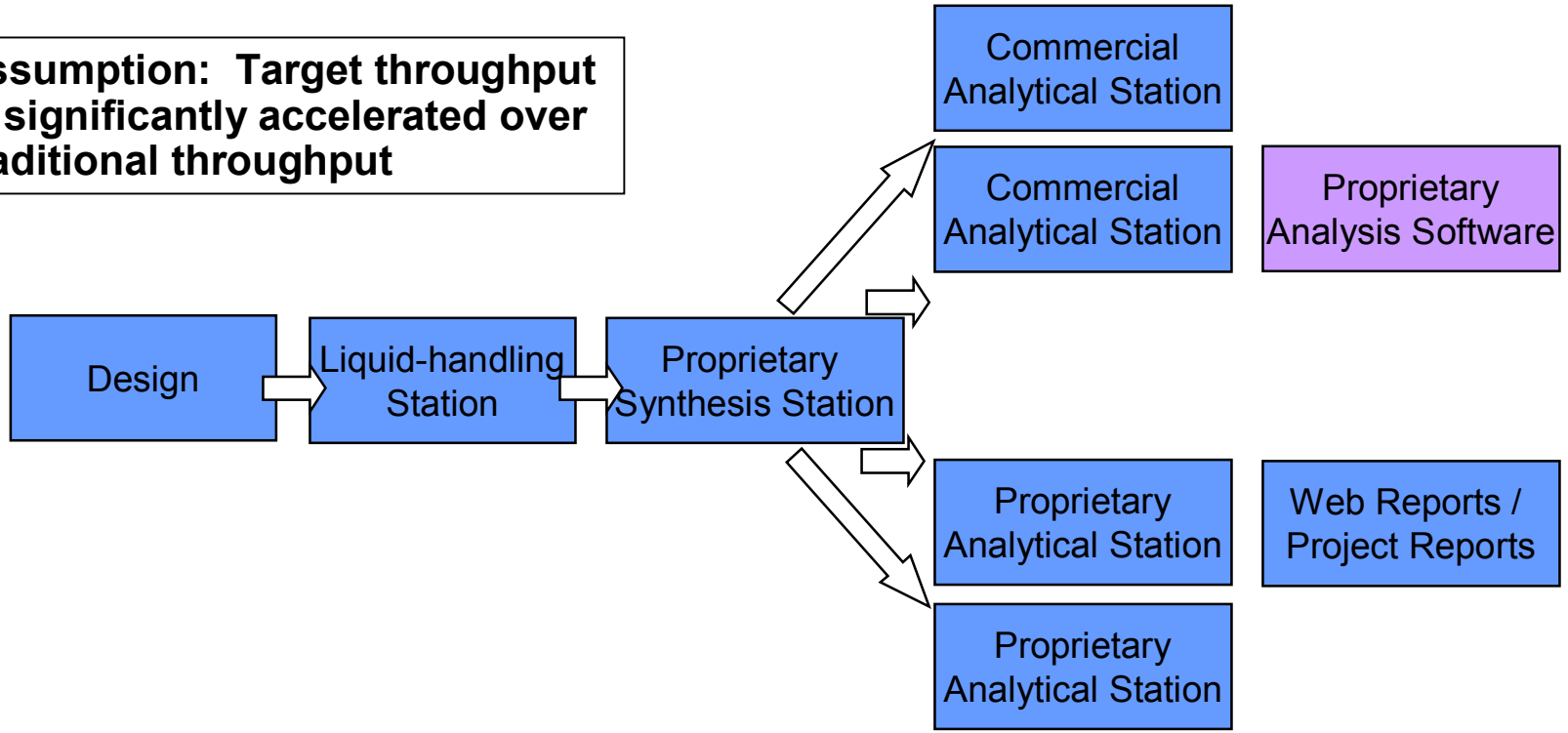
- Oracle / SQL
- Object-Relational Mapping
- Automation
- Database: Reporting, querying, chromatograms/xy datasets, images, numbers
- Client Applications / Web Applications
- Developer kit
- C++ / ATL / COM / XML / XSLT / JAVA / HTTP…

Existing Foundation:
100 person-years invested



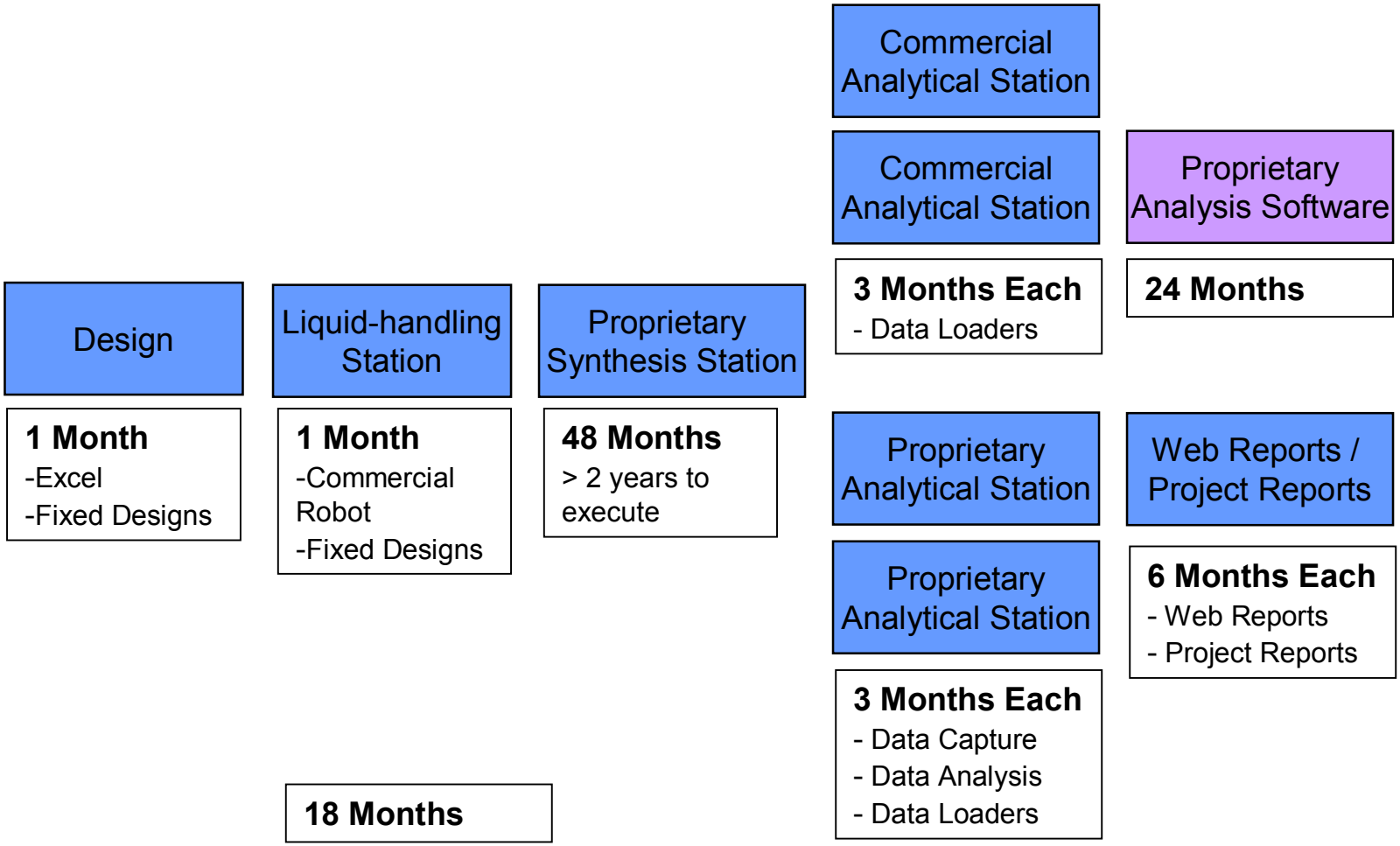
New Workflow – Informatics Blocks

Assumption: Target throughput is significantly accelerated over traditional throughput



Database: Track & Correlate data - #'s, images, xy data, chromatograms, etc.

New Workflow – Informatics Blocks



New Workflow – Informatics Implementation From Scratch

Software Implementation From Scratch:

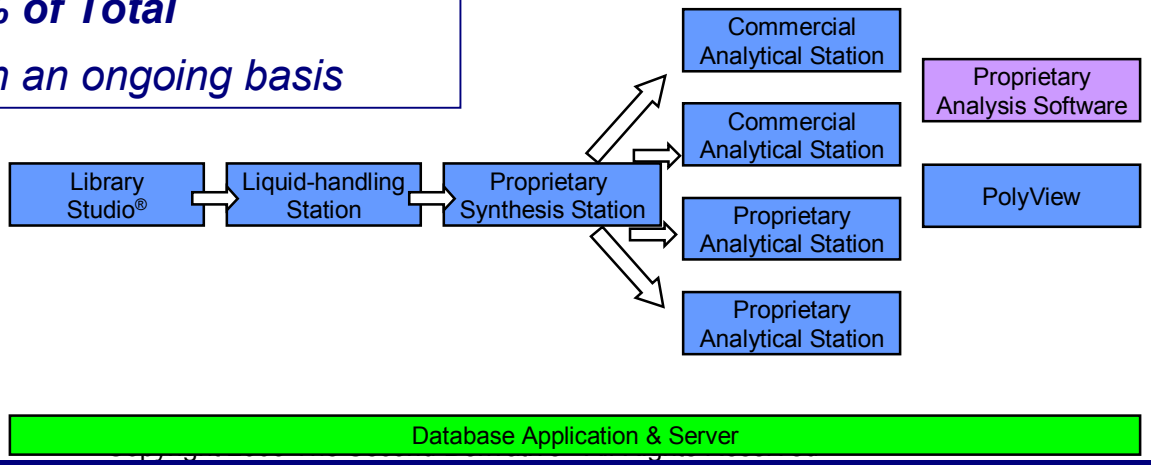
116 months (~10 person-years), over a period of 2-4 years

Staffing and Disciplines (SW Only):

? individual staff members
- Oracle / SQL
- Automation
- Database: Reporting, Querying, Chromatograms/xy datasets, images, numbers
- Client Applications / Web Applications
- C++ / ATL / COM / XML / XSLT / JAVA / HTTP…

Support ~20% of Total

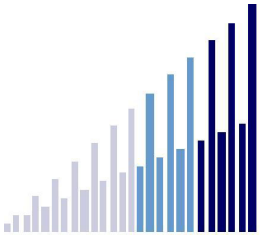
~1-2 people on an ongoing basis



New Workflow – Informatics Implementation From Scratch – Implications and Risks

Issues and Risks:

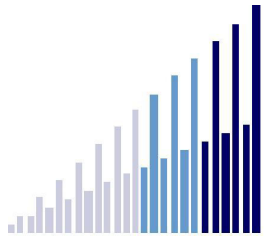
- Investment of people in core-vs.-context activities
  - 10 person-years to begin
  - 1-2 person-years ongoing
- Time-line to completion
- Risk of failure
- Initial cost estimates vs. true costs (“Are you in denial?”)
- Complexity beyond expectations
- Experience (or lack of) with large projects
- Uncertainly of workflow and methods
- Risk of data integrity
- Risk of data errors / erroneous data handling
- Lack of inter-project leverage
- Risk of ability to support on an ongoing basis



New Workflow – Pre-Summary Build vs. Buy

Costs to Build

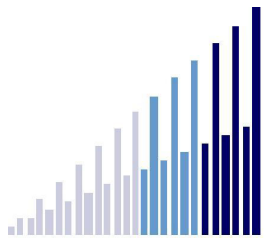
■ Hardware:	~$1.0M	~15-20%
■ Software:	~$2.5 - 3.0M	~40-50%
■ Engineering:	~$1.0M	~15-20%
■ Chemistry:	~$1.2M	~15-25%
Total:	~$5.7 – 6.2M	



Summary

- Evaluate business objectives:
  - Single project vs. many projects (Core or Context?)
  - Time to implement
- Evaluate the value of the workflow contemplated
  - Throughput, TTD, FTE's, etc.
- Evaluate Costs to Build and Support Over Lifetime
  - Hardware: 15-20% → $?
  - Software: 40-50% → $?
  - Engineering: 15-20% → $?
  - Chemistry: 15-20% → $?
  - Ongoing Support: ~20% of (HW, SW, ENG, CHEM)

  Total: $?

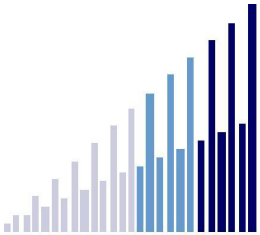


“Core” or “Context”?

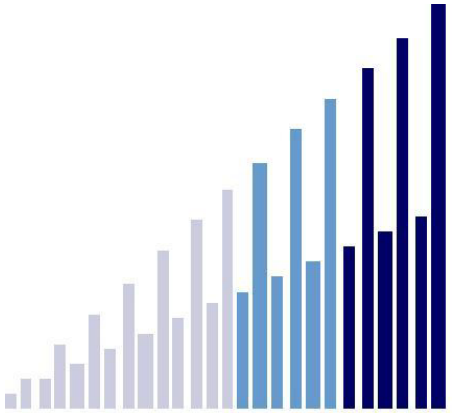
- Core: Stuff that makes your business what it is
- Context: Stuff that has to be done but does not really differentiate

- Moral:

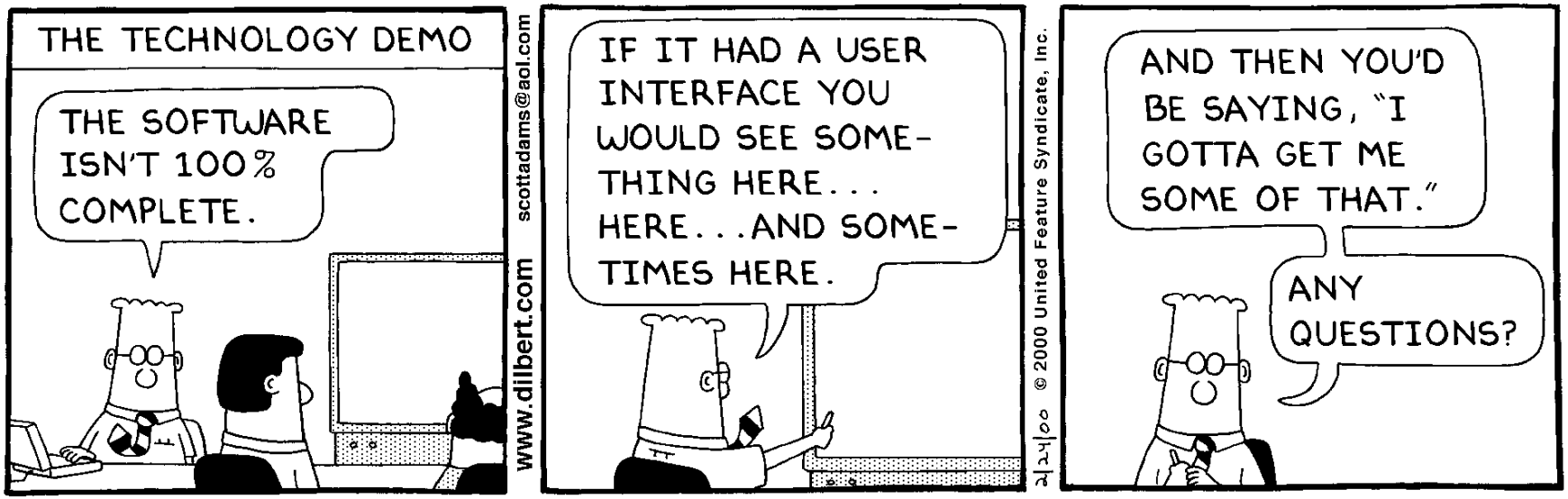
  Invest in “Core”, Outsource “Context”



Impact of Software Demonstrations



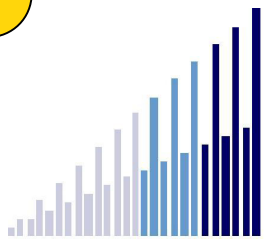
Demos…



DILBERT reprinted by permission of United Feature Syndicate, Inc.

A Great Demo

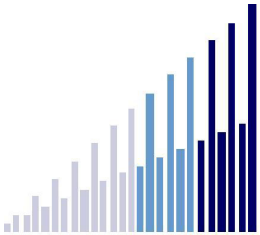
"***Do the Last Thing First!***"



A Great Demo

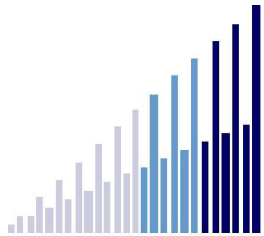
(Introduction)

1. Provide the Illustration - Summarize
2. Do it - Summarize
3. Do it again - Summarize
4. Questions & Answers
5. Summarize



How can demos go wrong?

- A feature failed – software bugs/crashes
- Failure to identify Critical Business Issues
- Demonstrator didn't know the product
- Unknown or unqualified audience needs
- Can't drive the message
- No story
- Confusing story
- Too long
- Too boring
- Too many features
- Didn't stop in time
- Unclear story
- Got lost in the story
- No point to the story
- No conclusion or poor conclusion
- Broad range of audience needs
- Disconnect between Sales and Technical
- Capabilities didn't match needs
- Lack of demo skills
- Lack of clear objectives for the demo
- Too little time
- Too much time
- Equipment failure
- Equipment unavailable
- Questions interrupted the flow
- People interrupted the flow



What bad things happen when demos fail?

Development

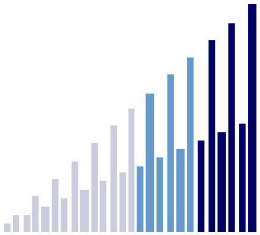
- Product capabilities are implemented poorly
- Wrong product built
- Wasted product development iterations
- Missed release dates

Deployment:

- User adoption is slowed or stalled
- Feedback cycle to vendor is attenuated – missed opportunities
- Training costs increase
- Professional services (consulting) costs increase
- Adoption is limited – “shelfware”
- Benefits delayed (ROI)

Sales

- Cost of sale increases
- Lost opportunities
- Value of sale is reduced
- Sales cycle is extended
- Sale is lost
- Fewer products/services sold
- Company misses quarterly or annual goals
- Salesperson misses quota
- Commission is lost or reduced
- People leave



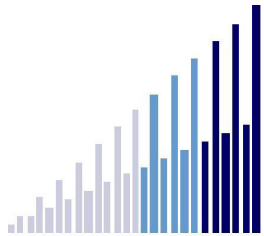
Why do you (or your customers) build or buy software?

Existing Problems or Business Issues:

- Existing Problem 1 → Solution
- Existing Problem 2 → Solution
- Existing Problem 3 → Solution

Anticipated Problems or Business Opportunities

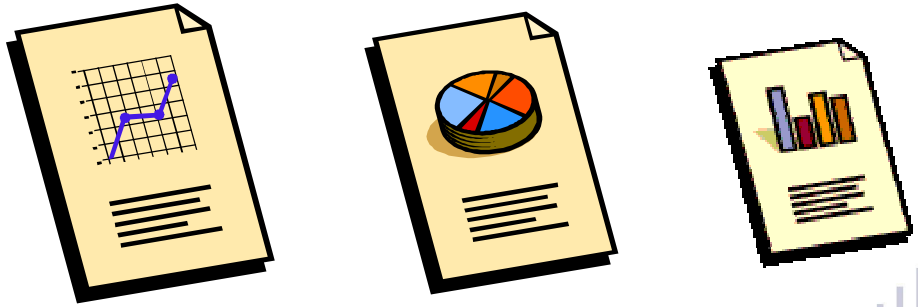
- Anticipated Problem → Solution
- New Opportunity → Realized



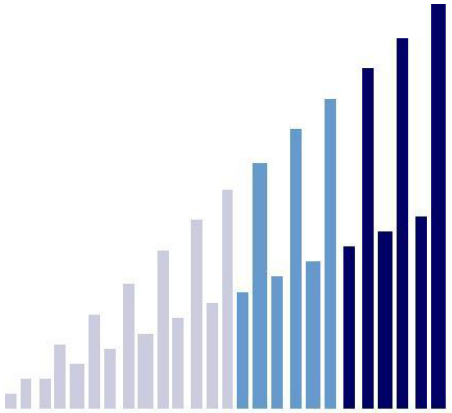
Solutions: What are the key capabilities provided by the software?

- Capability #1
  - Illustration
- Capability #2
  - Illustration
- Capability #3
  - Illustration
- Capability #4
  - Illustration

Solutions… that address a problem, an objective, or Critical Business Issue

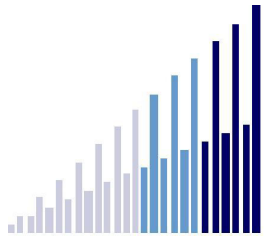


Developing a Great Demo….



What do you need to create a Great Demo?

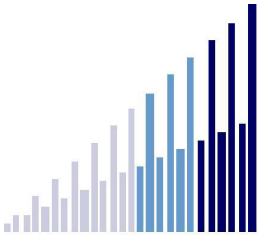
1. Objective
   - Proof of capabilities
   - Vision generation
2. Organization Chart
   - Audience members and roles
3. Critical Business Issues
   - CBI(s) and Specific Capabilities needed for each audience member
4. Infrastructure
   - When, where, how, who, with what…



Executing a Great Demo

(Introduction)

1. Provide the Illustration - Summarize
2. “Do it” - Summarize
3. “Do it again” - Summarize
4. Questions & Answers
5. Summarize

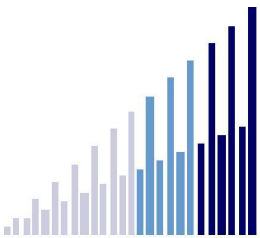


Some Comments About Collaborative Tools (WebEx and Similar…)

- Good alternative way to provide a demo
  - Reduces cost - travel and lost time on-the-road
- Most effective when a representative from your firm is present at the customer site (the demonstrator can be in California, via WebEx)
  - See the reaction of the audience
  - First-hand observations are important!
- Resist the urge to point at your own screen with your finger…!
  - I've SEEN this...! Shockingly, the customer can't see your hand…
- *Interactivity is the name of the game*

Summary

- Some Definitions of “Integration”
  - ✍ Beauty, Workflows, and Integration are in the eye of the beholder…
- HT Workflow Value Analysis
  - 👍 ROI is terrific
- Workflow Software Build vs. Buy Analysis
  - ☞ Invest in “Core”, Outsource “Context”
- Improving Demonstrations
  - ☝ Do the Last Thing First!

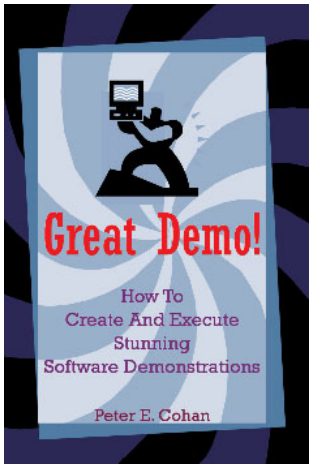


The Second Derivative

The Second Derivative
helps software organizations improve their sales and marketing results by helping folks with demonstration and presentation skills, value analyses, pricing, and related thorny problems.

"Do the Last Thing First!"

Contact Information
Peter E. Cohan
Principal
The Second Derivative
1538 Winding Way
Belmont, CA 94002
Telephone: +1 650 631 3694
Email: P.Cohan@comcast.net



"Great Demo!" is available on www.Amazon.com, www.BarnesandNoble.com, and directly from the author