Software engineering for HPC

Paolo Ciancarini - paolo.ciancarini@unibo.it
Department of Informatics - University of Bologna
Agenda

- What is Software Engineering?
- The Iterative Development Lifecycle
- Software Development Activities
- Methods and tools
- Software processes
Using software in a research project

Your Project

Publications

Data

Software

Used by other projects

Other software
What is the future of your software?
A survey on scientists using HPC

- Scientists use more than 40% of their time using or building software
- 96% are self-taught
- No data on how well they do things (only 47% know the basics of testing)
- No data on how much software they reuse, or produce that is reused

[G. Wilson, Software Carpentry]
HPC

- Usage of supercomputers or advanced computing systems in solving complex scientific problems based on computationally intensive tasks
- It includes using
  - Infrastructure
    - HPC hardware architectures
    - Interconnection network
    - Operating systems and middleware
  - Parallel programming
    - Languages
    - Algorithms
HPC developers

- The majority of the HPC developers are not sw engineers or computer scientists
- Primary goal of HPC developers: computational science
  - Achieving scientific results in some field of research using HP computers
- Hence, most HPC users build software, but almost all of them lack formal software engineering knowledge
HPC developers

- Most computational scientists learn software development from mentors or peers within their disciplines
  - Little or no formal training in computer science; informal “self-study” of programming and software development is variable
  - Reward structure favors communicating *scientific* results, not the *software* that enabled the results
  - the software is often the basis of a competitive advantage
  - Horizontal knowledge transfer diffusion is slow
Typical software development in HPC

What happens to the software?

- Thrown away
- Kept on some systems, possibly in different versions
- Dumped on a code repository

What happens when...
- You have a follow-on project?
- Someone wants to (re)use the code?
- Someone wants to reproduce your results?
- Maintenance or future reuse should be considered?
Beware of software aging!

Software can *age*

- Ill-conceived modifications
- Functional operation degrades over time
- It becomes unsustainable, unusable
- Lack of proper maintenance
- Infrastructure (os, libraries, language platform) evolves
- Some software types more susceptible
Enters Software Engineering

“Software engineering is the discipline concerned with all aspects of software production from the early stages of system specification to maintaining the system after it has gone into use”

[Sommerville 2007]
Software Engineering

“The establishment and use of sound engineering principles in order to obtain economically software that is reliable and works efficiently on real machines.” [Naur & Randell, 1968]
What is Software Engineering?

A naive view:

Problem Specification \[ \rightarrow \text{coding} \rightarrow \text{Final Program} \]

But …

- Where did the *problem specification* come from?
- How do you know the problem specification corresponds to and satisfies the *user’s needs*?
- How did you decide how to *structure* your program?
- How do you know the program actually *meets the specification*?
- How do you know your program will always *work correctly*?
- What do you do if the users’ *needs change*?
- How do you *divide tasks up* if you have more than a one person in the developing team?
- How do you *reuse* existing software for solving similar problems?
Software Engineering

- Some definitions and issues
  - “state of the art of developing quality software on time and within budget”
- Trade-off between a system perfectly engineered and the available resources
  - SE has to deal with real-world issues
- State of the art
  - Community decides on “best practice” + life-long education
What is Software Engineering?

“multi-person construction of multi-version software”

— Parnas

- Team-work
  - Scale issue ("program well" is not enough)
    + Communication Issue
- Successful software systems must evolve or perish
  - Change is the norm, not the exception
What is Software Engineering?

“software engineering is different from other engineering disciplines”
— Sommerville

- Not constrained by physical laws
  - limit = human knowledge
- It is constrained by social forces
  - Balancing stake-holders needs
  - Consensus on functional and especially non-functional requirements
Software Engineering

- Software engineering is ... dedicated to designing, implementing, and modifying software so that it is of higher quality, more affordable, maintainable, and faster to build.

- The application of a systematic, disciplined, quantifiable approach to the development, operation, and maintenance of software; that is, the application of engineering to software [Guide to the Software Engineering Body of Knowledge]
Roadmap

- What is Software Engineering?
- The Iterative Development Lifecycle
- Software Development Activities
- Methods and tools
- Software processes
## Software Development Activities

<table>
<thead>
<tr>
<th>Requirements Collection</th>
<th>Establish customer’s needs</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Analysis</strong></td>
<td>Model and specify the requirements (“what”)</td>
</tr>
<tr>
<td><strong>Design</strong></td>
<td>Model and specify a solution (“how”)</td>
</tr>
<tr>
<td><strong>Implementation</strong></td>
<td>Construct a solution in software</td>
</tr>
<tr>
<td><strong>Testing</strong></td>
<td>Validate the software against its requirements</td>
</tr>
<tr>
<td><strong>Deployment</strong></td>
<td>Making a software available for use</td>
</tr>
<tr>
<td><strong>Maintenance</strong></td>
<td>Repair defects and adapt the sw to new requirements</td>
</tr>
</tbody>
</table>

*NB: these are ongoing activities, not sequential phases!*
First development step: requirements

- The first step in any development process consists in understanding the needs of someone asking for a software.
- The needs should be stated explicitly in “requirements”, which are statements requiring some function or property to the final software system.
A Software Requirement is … (IEEE 610)

1) A condition or capability needed by a user to solve a problem or achieve an objective
2) A condition or capability that must be met or possessed by a system or component to satisfy a contract, standard, specification, or other formally imposed documents
3) A documented representation of a condition or capability as in (1) or (2)
The requirements pyramid

Some user has some need

Needs are answered by “features” that some system must have

Each feature corresponds to a need and is a collection of requirements

Features and requirements can be aggregated in “scenarios” where testing can prove that the features will satisfy the needs

Sw requirement specification

- An SRS document is an organization’s understanding of the requirements and dependencies of some system.
- It is written (usually) prior to any actual design or development work.
- It is a two-way insurance policy that assures that both the client and the organization understand the other’s requirements from that perspective at a given point in time.
- The SRS document itself states those functions and capabilities a software system (e.g., an app, an eCommerce Web site, etc) must provide, as well as it states any required constraints by which the system must abide.
Requirements and tests

User requirements
  Test reqs
  Scenarios and test cases
  Test script
The classical software lifecycle models the software development as a step-by-step “waterfall” between the various development phases.

The waterfall model is unrealistic for many reasons:

- Requirements must be *frozen too early* in the life-cycle
- Requirements are *validated too late*
- Risks in constructing wrongly the software are high
Problems with the waterfall lifecycle

1. “Real projects rarely follow the sequential flow that the waterfall model proposes. *Iteration* always occurs and creates problems in the application of the paradigm”

2. “It is often *difficult* for the customer to state all requirements explicitly. The classic life cycle requires this and has difficulty accommodating the natural uncertainty that exists at the beginning of many projects.”

3. “The customer must have patience. A *working version* of the program(s) will not be available until *late in the project* timespan. A major blunder, if undetected until the working program is reviewed, can be disastrous.”

   — Pressman, SE, p. 26
Iterative Development

In practice, development is always iterative, and *most* activities can progress in parallel.

If the waterfall model is pure fiction, why is it still the dominant software process?
Iterative Development

- Plan to iterate your analysis, design and implementation
  - You will not get it right the first time, so integrate, validate and test as frequently as possible
  - During software development, more than one iteration of the software development cycle may be in progress at the same time
  - This process may be described as an 'evolutionary acquisition' or 'incremental build' approach
Incremental Development

Plan to *incrementally* develop (i.e., prototype) the system

- If possible, *always have a running version* of the system, even if most functionality is yet to be implemented
- *Integrate* new functionality as soon as possible
- *Validate* incremental versions against user requirements.
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User requirements are often expressed *informally*:

- features
- usage scenarios

Although requirements may be documented in written form, they may be *incomplete, ambiguous*, or *incorrect*
Changing requirements

Requirements *will* change!

- *inadequately captured* or expressed in the first place
- user and business *needs may change* during the project

Validation is needed *throughout* the software lifecycle, not only when the “final system” is delivered!

- build constant *feedback* into your project plan
- plan for *change*
- early *prototyping* [e.g., UI] can help clarify requirements
Requirements Analysis

Analysis is the process of specifying what a system will do.

- The goal is to provide an understanding of what the system is about and what its underlying concepts are.

The result of analysis is a specification document.

Does the requirements specification correspond to the users’ actual needs?
Object-Oriented Analysis

An *object-oriented analysis* results in models of the system which describe:

- **classes** of objects that exist in the system
  - *responsibilities* of those classes
- **relationships** between those classes
- **use cases** and **scenarios** describing
  - *operations* that can be performed on the system
  - allowable *sequences* of those operations
Prototyping

A **prototype** is a software program developed to test, explore or validate a hypothesis, i.e. *to reduce risks*

An **exploratory prototype**, also known as a **throwaway prototype**, is intended to **validate requirements** or **explore design choices**

- UI prototype — validate user requirements
- rapid prototype — validate functional requirements
- experimental prototype — validate technical feasibility
Prototyping

An *evolutionary prototype* is intended to evolve in steps into a finished product.

- iteratively “grow” the application, *redesigning* and *refactoring* along the way

*First do it, then do it right, then do it fast.*
Design is the process of specifying how the specified system behaviour will be realized from software components. The results are architecture and detailed design documents.

Object-oriented design delivers models that describe:

- how system operations are implemented by interacting objects
- how classes refer to one another and how they are related by inheritance
- attributes and operations associated to classes

Design is an iterative process, proceeding in parallel with implementation!
Conway’s Law

- The law: *Organizations that design systems are constrained to produce designs that are copies of the communication structures of these organizations*
- Example: "If you have four groups working on a compiler, you'll get a 4-pass compiler"
- Several studies found significant differences in modularity when software is outsourced, consistent with a view that distributed teams tend to develop more modular products
Implementation and Testing

*Implementation* is the activity of *constructing* a software solution to the customer’s requirements.

*Testing* is the process of *validating* that the solution meets the requirements.

- The result of implementation and testing is a *fully documented* and *validated* solution.
Testing, Testing!

1. Provide automated build process
   - Far easier & quicker to validate changes
   - e.g. Make, Ant, Maven

2. Provide automated regression test suite - TDD
   - Do changes break anything?
   - JUnit, CPPUnit, xUnit, fUnit, …

3. Join together: automated build & test
   - A ‘fail-fast’ environment

4. Infrastructure support
   - Nightly builds – run build & test overnight, send reports
   - Continuous integration - run build & test when codebase changes

Towards anytime releasable code!
Design, Implementation and Testing

Design, implementation and testing are iterative activities

- The implementation does not “implement the design”, but rather the design document documents the implementation!

- System tests reflect the requirements specification
- Testing and implementation go hand-in-hand
  - Ideally, test case specification precedes design and implementation
Maintenance is the process of changing a system after it has been deployed.

- **Corrective maintenance**: identifying and repairing defects
- **Adaptive maintenance**: adapting the existing solution to new platforms
- **Perfective maintenance**: implementing new requirements
- **Preventive maintenance**: repairing a software product before it breaks

In a spiral lifecycle, everything after the delivery and deployment of the first prototype can be considered “maintenance”!
Maintenance activities

“Maintenance” entails:

- configuration and version management
- reengineering (redesigning and refactoring)
- updating all analysis, design and user documentation

Repeatable, automated tests enable evolution and refactoring
"Maintenance" typically accounts for 70% of software costs!

Means: most project costs concern continued development after deployment

– Lientz 1979
Configuration management

- Run your own CM system, if you have the resources
  - Generally easy to set up
  - Full control, but be sure to back it up!
- Some public solutions can offer most of these for free
  - SourceForge, GoogleCode, GitHub, Codeplex, Launchpad, Assembla, Savannah, …
  - BitBucket for private code base (under 5 users)
  - See (for hosting code and related tools)
    http://software.ac.uk/resources/guides/choosing-repository-your-software-project
  - See (for hosted continuous integration)
    http://www.software.ac.uk/blog/2012-08-09-hosted-continuous-integration-delivering-infrastructure

“If you’re not using version control, whatever else you might be doing with a computer, it’s not science” – Greg Wilson, Software Carpentry
Deployment

- Virtual Machines
  - Software pre-installed, ready to run
  - Often easiest
  - Not enough in itself – documentation!

- Release software
  - Prioritise & select requirements -> Develop -> Test -> Commit changes to repository -> Test -> Release
  - Documentation (minimum: quick start guide)

- Licencing
  - Specify rights for using, modifying and redistributing
Roadmap

- What is Software Engineering?
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- Software Development Activities
- Methods and tools
- Software processes
Principles, methods and tools

**Principle** = general statement describing desirable properties

**Method** = general guidelines governing some activity

**Technique** = more technical and mechanical than method

**Methodology** = package of methods and techniques packaged

— Ghezzi et al. 1991
Object-Oriented Methods: a short history

First generation:
- Adaptation of existing notations (ER diagrams, state diagrams ...): Booch, OMT, Shlaer and Mellor, ...
- Specialized design techniques:
  - CRC cards; responsibility-driven design; design by contract

Second generation:
- Fusion: Booch + OMT + CRC + formal methods

Third generation:
- Unified Modeling Language:
  - uniform notation: Booch + OMT + Use Cases + ...
  - various UML-based methods (e.g. Catalysis)
UML is a modeling language

- A modeling language allows the specification, the visualization, and the documentation of the development of a software system
- The models are artifacts which clients and developers use to communicate
- UML 1.* is a modeling language
- UML 2.* is also a programming language
Meaning of models for software

- A model is a *description* of the structure and meaning of a system
- A model is always an *abstraction* at some level: it captures the essential aspects of a system and ignores some details
- NB: a model can be also *generator* of potential *configurations* of systems
Class diagram: example

**Order**
- **dateReceived**: Date[0..1]
- **isPrepaid**: Boolean[1]
- **number**: String[1]
- **price**: Money

**Order line**
- **quantity**: Integer
- **price**: Money

**Product**

**Customer**
- **name**: String[1]
- **address**: String[0..1]
- **getCreditRating()**: String

**Corporate Customer**
- **contactName**
- **creditRating**
- **creditLimit**

**Personal Customer**
- **creditCardNumber**

**Employee**
- **salesRep**: String[0..1]

**Class name**
**Attributes**
**Operation**
**Generalization**
**Multiplicity**
**Role name**
**Constraint**
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Software: the product of a process

- Many kinds of software products → many kinds of development processes
- “Study the process to improve the product”

- A software development process can be described according to some specific “model”
- Examples of process models: waterfall, iterative, agile, extreme,…
- The models differ mainly in the roles and activities that the stakeholders cover
The production of software in the contemporary world

- Centralized vs distributed (offshore)
- Code centric vs data intensive
- In lab vs in the large
- Long planned vs continuous release
- Single system vs product lines
- Stakeholders: community vs market
Stakeholders

Typical stakeholders in a sw process

- Designers
- Management
- Technicians
- Decisors
- Users
- Funding people
- ...

Each stakeholder has a specific viewpoint on the product and its development process
# HPC stakeholders attributes

<table>
<thead>
<tr>
<th>Attribute</th>
<th>Values</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Team size</td>
<td>Individual</td>
<td>This scenario, sometimes called the &quot;lone researcher&quot; scenario, involves only one developer.</td>
</tr>
<tr>
<td>Code life</td>
<td>Large</td>
<td>This scenario involves “community codes” with multiple groups, possibly geographically distributed.</td>
</tr>
<tr>
<td>Code life</td>
<td>Short</td>
<td>A code that’s executed few times (for example, one from the intelligence community) might trade less development time (less time spent on performance and portability) for more execution time.</td>
</tr>
<tr>
<td>Code life</td>
<td>Long</td>
<td>A code that’s executed many times (for example, a physics simulation) will likely spend more time in development (to increase portability and performance) and amortize that time over many executions.</td>
</tr>
<tr>
<td>Users</td>
<td>Internal</td>
<td>Only developers use the code.</td>
</tr>
<tr>
<td>Users</td>
<td>External</td>
<td>The code is used by other groups in the organization (for example, at US government labs) or sold commercially (for example, Gaussian, <a href="http://www.gaussian.com">www.gaussian.com</a>)</td>
</tr>
<tr>
<td>Users</td>
<td>Both</td>
<td>“Community codes” are used both internally and externally. Version control is more complex in this case because both a development and a release version must be maintained.</td>
</tr>
</tbody>
</table>
Lifecycles

- Lifecycles are created and adapted to different products
- Both products and lifecycles can be evaluated for their quality
- Software needs several different lifecycle layers:
  - Industrial lifecycle
  - Development lifecycle (reqs, design, build, test)
  - Operational lifecycle (eg.: portal)
The software development process

- **Software process**: set of roles, activities, and artifacts necessary to create a software product
- Possible **roles**: designer, developer, tester, maintenance, ecc.
- Possible **artifacts**: source code, executables, specifications, comments, test suite, etc.
Activities

- Each organization differs in products it builds and the way it develops them; however, most development processes include:
  - Specification
  - Design
  - Verification and validation
  - Evolution

- The development activities must be modeled to be managed and supported by automatic tools
Control variables of sw processes

- Time – duration of the project
- Quality – satisfying the stakeholders
- Resources – personnel, equipment, etc.
- Scope – what is to be done; the features to be implemented

These control variables are very difficult to control all; the simplest and most effective to control is scope

The theory of software process models has the goal of controlling the other variables as well
Models for the software process

- Waterfall (planned, linear)
- Spiral (planned, iterative)
- Agile (unplanned, test driven)
Traditional process model

- Waterfall

Diagram showing the stages of the Waterfall model:
- Requirements
- Design
- Code
- Test
- Deploy
Waterfall characteristics

- Delays confirmation of critical risk resolution
- Measures progress by assessing work-products that are poor predictors of time-to-completion
- Delays and aggregates integration and testing
- Precludes early deployment
- Frequently results in major unplanned iterations
The Spiral Lifecycle (B. Bohem)

Planning = determination of objectives, alternatives and constraints

Risk Analysis = Analysis of alternatives and identification/resolution of risks

Risk = something that will delay project or increase its cost

go, no-go decision

first prototype

Customer Evaluation = Assessment of the results of engineering

Evolving system

Engineering = Development of the next level product
A process for HPC [Lugato 2010]
Iterative Development

- **Phase** - the time between two major project milestones, during which a well-defined set of objectives is met, artifacts are completed, and decisions are made to move or not into the next phase. A phase includes one or more iterations.

- **Iteration** – a time period in which a number of predefined tasks are performed and results are evaluated to feedback to the next iteration. An iteration results in a release.

- **Release (external)** – a coherent set of completed functionalities (code and other artifacts) that is useful to the stakeholders of the system

- **Release (internal)** - a coherent set of completed functionalities that is used only by the development organization, as part of a milestone, or for a demonstration to users
Test each iteration

UML Model and Implementation

Tests

Iteration 1

Iteration 2

Iteration 3

Iteration 4

Test Suite 1

Test Suite 2

Test Suite 3

Test Suite 4
RUP is iterative

Original RUP
Benefits of Iterative Development

A software project evolves in iterations to:

- Mitigate risk
- Accommodate change
- Learn along the way
- Improve the quality of the artifacts
- Exploit reuse thus increasing productivity
Committed vs involved

- The core roles in development teams are those **committed** to the project in the process - they are the ones producing the product: product owner, team, project manager.

- The other roles in teams are those with no formal role and **infrequent involvement** in the process - and must nonetheless be taken into account.
A pig and a chicken are walking down a road. The chicken looks at the pig and says, "Hey, why don't we open a restaurant?" The pig looks back at the chicken and says, "Good idea, what do you want to call it?" The chicken thinks about it and says, "Why don't we call it 'Ham and Eggs'?" "I don't think so," says the pig, "I'd be committed but you'd only be involved."
Agile ethics

- www.agilemanifesto.org

We are uncovering better ways of developing software by doing it and helping others do it. Through this work we have come to value:

- **Individuals and interactions** over **processes and tools**
- **Working software** over **comprehensive documentation**
- **Customer collaboration** over **contract negotiation**
- **Responding to change** over **following a plan**

That is, while there is value in the items on the right, we prefer the items on the left.

- **Management can tend to prefer the things on the right over the things on the left**
Traditional vs agile team

**Traditional Silos**
- Product Owner
- PM
- BA
- Designer
- Developer
- Tester

**Integrated Agile Team**
- Core Project Team
  - Release Manager
  - Architect
  - DBA
  - Product Owner
  - Risk Assessor
  - Developer
  - Developer
  - Product Owner
  - Tech Ops
  - Business Sponsor
  - Security
  - Extended Project Team
    - PM
    - BA
    - Capacity Planner

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Agile development uses feedback to make constant adjustments in a highly collaborative environment.

There are many agile development methods; most minimize risk by developing software in short amounts of time.

Software developed during one unit of time is referred to as an *iteration*, which typically lasts from hours or few days.

Each iteration passes through a full software development cycle.
The Generic Agile Lifecycle

Start work on release N+1

**Iteration 0 (Warm Up)**
- Initiate the Project

**Development Iterations**
- Deliver a working system which meets the changing needs of stakeholders

**Release (End Game)**
- Deploy Release N into Production

**Production**
- Operate and Support Release N

- Active stakeholder participation
- Obtain funding and support
- Start building the team
- Initial requirements envisioning
- Initial architecture envisioning
- Setup environment
- Active stakeholder participation
- Collaborative development
- Model storming
- Test driven design (TDD)
- Confirmatory testing
- Evolve documentation
- Internally deploy software
- Active stakeholder participation
- Final system testing
- Final acceptance testing
- Finalize documentation
- Pilot test the release
- Train end users
- Train production staff
- Deploy system into production

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Agile practices

Test-Driven Design (TDD)

Iteration Modeling

Executable Specifications

Document Late

Single Source Information

Multiple Models

Requirements Envisioning

Just Barely Good Enough

Model Storming

Architecture Envisioning

Prioritized Requirements

Active Stakeholder Participation

Model a bit Ahead

The Best Practices of Agile Modeling

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Agile Unified Process

Phases

- Inception
- Elaboration
- Construction
- Transition

- Model
- Implementation
- Test
- Deployment
- Configuration Management
- Project Management
- Environment

Iterations

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Team-Level Planning

Every 24hrs

Prioritised Iteration Scope

Every Iteration 4-6 weeks

Working Software Delivered

Prioritised Requirements & Features “Backlog”

Applying Agile:
Continuous integration; continuously monitored progress

Daily Scrum Meeting:
15 minutes
Each team member answers 3 questions:
1) What did I do since last meeting?
2) What obstacles are in my way?
3) What will I do before next meeting?
Agile: eXtreme Programming

The ethic values of eXtreme Programming
- Communication
- Simplicity
- Feedback
- Courage
- Respect (added in the latest version)
eXtreme Programming (XP)

- “Extreme Programming is a discipline of software development based on values of simplicity, communication, feedback, and courage”
- Proponents of XP and agile methodologies regard ongoing changes to requirements as a natural and desirable aspect of sw projects
- They believe that adaptability to changing requirements at any point during the lifecycle is a better approach than attempting to define all requirements at the beginning and then expending effort to control changes to the requirements

www.extremeprogramming.org
The 12 Practices of XP

1. Metaphor
2. Release Planning
3. Testing
4. Pair Programming
5. Refactoring
6. Simple Design
7. Collective Code Ownership
8. Continuous Integration
9. On-site Customer
10. Small Releases
11. 40-Hour Work Week
12. Coding Standards
Conclusions

Software engineering deals with

- the way in which software is made (process),
- the languages to model and implement software,
- the tools that are used, and
- the quality of the result (testing)
Self test questions

- How does Software Engineering differ from programming?
- Why is the “waterfall” model unrealistic?
- What is the difference between analysis and design?
- Why plan to iterate? Why develop incrementally?
- Why is programming only a small part of the cost of a “real” software project?
- What are the key advantages and disadvantages of object-oriented methods?
References: books

  www.computer.org/portal/web/swebok
Reference: papers

Useful sites

- software-carpentry.org  Software carpentry
- software.ac.uk/resources/case-studies
- First Int. Workshop on Sw eng for HPC, 2013 sehpccse13.cs.ua.edu
Questions?

[Image of a flowchart titled "How to Write Good Code:"]

- Start project.
- Do things fast or do them right?
  - Fast
  - Code fast
  - Does it work yet?
    - No
    - Almost, but it's become a mass of kludges and spaghetti code.
    - No, and the requirements have changed.
    - Throw it all out and start over.
  - Right
    - Code well
    - Are you done yet?
      - No
      - Good code.