

Basic concepts of software engineering and maintenance

G. Giuliani International Centre for Theoretical Physics -
Trieste Earth System Physics Section

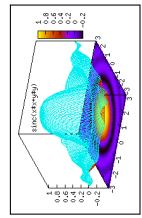
ICTP - Earth System Physics Section

Advanced School on Scientific Software Development
Trieste, 20 Feb - 2 Mar 2012



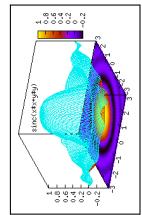
Is Software part of Science?

- What Science is About



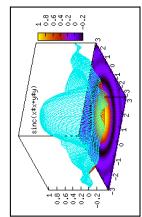
Is Software part of Science?

- What Science is About
 - Try to understand Reality



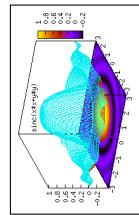
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 - Collect information as numerical values



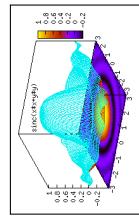
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 - Try to understand Reality
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 - Build knowledge on it with analysis and models



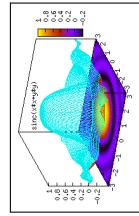
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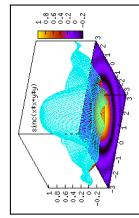
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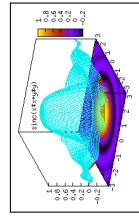
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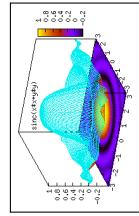
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 - Software development is not science for itself



The Scientifical Problem

- The Scientist aims to understand the reality



The Scientifical Problem

- ▶ The Scientist aims to understand the reality
- ▶ The Scientist makes models of the reality



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 - ▶ The model is a bunch of math equations



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 - ▲ The software is the instruction to get there
 - ▲ If the time to result is lowered by calculator
 - ▲ The Scientist is happy with publications



The Software

- Software for science is...



The Software

- Software for science is...
 - Data Digitalization and Storage



The Software

- Software for science is...
 - ▲ Data Digitalization and Storage
 - ▲ Numerical Algorithms and Packages



The Software

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 - Information Exchange Systems



My Problem needs a new solution

- I need to write software if



My Problem needs a new solution

- ▶ I need to write software if
 - ▶ I have a new instrument



My Problem needs a new solution

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 - I have a new numerical algorithm
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 - I have a new community to share data with
- Is there a Good Way to write Scientific Software ?



The wrong way of writing scientific software

- I will just have to do it once



The wrong way of writing scientific software

- I will just have to do it once
- Nobody cares on how I do get to the answer, I will never share this with others



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- ▶ The resources I have is what everybody have
- ▶ The data format is secondary, I know what they are
- ▶ The precision I need in result is the one the computer uses
- ▶ Software professionals are just overstimulated freaks



The Scientist as a programmer

- ▶ Poor knowledge of the Hardware



The Scientist as a programmer

- ▶ Poor knowledge of the Hardware
- ▶ Poor knowledge of the System Software



The Scientist as a programmer

- ▶ Poor knowledge of the Hardware
- ▶ Poor knowledge of the System Software
- ▶ Poor knowledge of the Tools



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- ▶ Poor knowledge of the System Software
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- ▶ Usually little money but lot of manpower



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- ▶ Poor knowledge of the System Software
- ▶ Poor knowledge of the Tools
- ▶ Usually little money but lot of manpower
- ▶ Usually forced to someone else best choices
- ▶ Very conservative, low sharing attitude



Software Engineering

- Design solution under constraint



Software Engineering

- ▶ Design solution under constraint
 - ▶ Understanding the computer



Software Engineering

- Design solution under constraint
 - Understanding the computer
 - Understanding the problem



Software Engineering

- Design solution under constraint
 - Understanding the computer
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 - Fit the two together and choose the right tools



Software Engineering

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 - Standards in both coding and data



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Software Engineering

- Design solution under constraint
 - Understanding the computer
 - Understanding the problem
 - Fit the two together and choose the right tools
 - Standards in both coding and data
 - Documentation of code and algorithm
 - Test on different platforms
 - Check possible failures
 - Whenever possible, seek for help



Understand the computer

- Mathematic is declarative (What is knowledge)



Understand the computer

- ▶ Mathematic is declarative (What is knowledge)
- ▶ Computer Science is imperative (How to knowledge)



Understand the computer

- ▶ Mathematic is declarative (What is knowledge)
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- ▶ We need a language to describe process



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 - ▲ Floating Point Arithmetic



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 - ▶ Read David Goldberg Paper What every computer scientist should know about floating-point arithmetic



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- ▶ Floating Point Arithmetic
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- ▶ Computer resources: economics of the calculation



Understand the problem

- Think with Data Structures



Understand the problem

- ▶ Think with Data Structures
 - ▶ Design Data Structures and access functions to them



Understand the problem

- Think with Data Structures
 - Design Data Structures and access functions to them
 - Design the program as a sequence of operations on data



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Understand the problem

- ▶ Think with Data Structures
 - ▶ Design Data Structures and access functions to them
 - ▶ Design the program as a sequence of operations on data
 - ▶ Design them to be expandable
- ▶ Design a flow diagram of the program and write it down



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 - ▶ Use standard tools if available (UML)



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 - ▶ Use standard tools if available (UML)
 - ▶ Use anyway the pseudocode
- ▶ Evaluate the requirements for the execution



Why You should follow coding standard

- You can understand Your own programs



Why You should follow coding standard

- You can understand Your own programs
- Someone else can understand Your own programs



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- You can have external contribution You understand



Why You should follow coding standard

- You can understand Your own programs
- Someone else can understand Your own programs
- You can have external contribution You understand
- You spare time in the long run: Science must be reproducible



Why You should use a revision control system

- ▶ You can follow the development of the program



Why You should use a revision control system

- You can follow the development of the program
- You can develop the program in a team



Why You should use a revision control system

- You can follow the development of the program
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Why You should use a revision control system

- ▶ You can follow the development of the program
- ▶ You can develop the program in a team
- ▶ You can revert the modifications done at any time
- ▶ You can calculate easily efforts required



Why You should plan testing

- ▶ You should test Your program for valid and invalid input



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- ▶ You want to have a way to test it again in the future



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- ▶ You want simple tools to follow program flow



Why You should have a Software Forge

- What is a Collaborative Development Environment?



Why You should have a Software Forge

- ▶ What is a Collaborative Development Environment?
 - ▶ Web based collaboration site



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 - Bugs tracking and ticketing



Scientific codebases

- ▶ Is writing from scratch always worth the task?



Scientific codebases

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- ▶ Mix of public domain, free software and commercial solutions



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Scientific codebases

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- ▶ Mix of public domain, free software and commercial solutions
- ▶ Commercial environments and tools for research: more the possible outcome, more the commercial
- ▶ Which policy should be used to develop scientific software?



Thank You !

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Scientific Software
Software Engineering
Instruments



ICTP - ESP Basic concepts of software engineering and maintenance