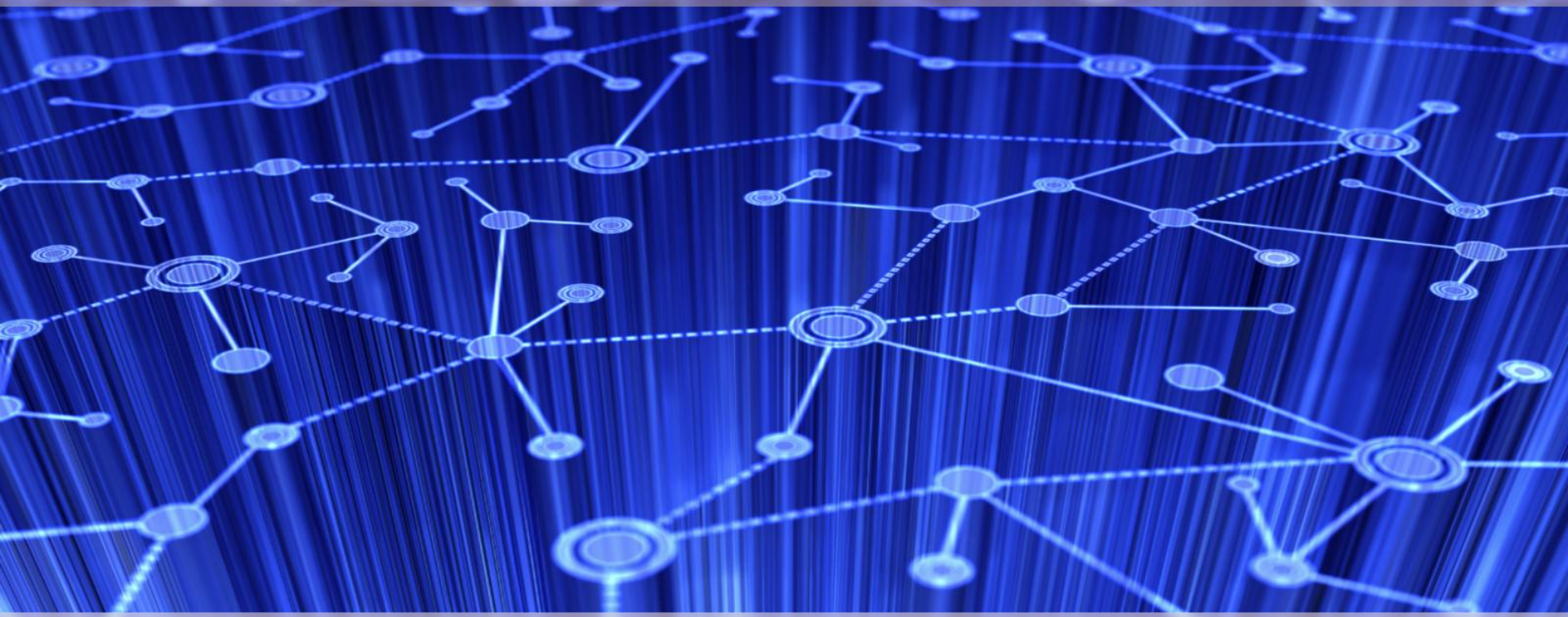


Foundations of High Performance Computing

Code optimization

Part I - There's no spoon

There is no spoon

Premature optimization is the root of all evil

D. Knuth

The rules of optimization club:

1. Don't talk about optimization
2. DON'T TALK ABOUT OPTIMIZATION *yet*
3. If your code yells stop, goes limp, taps out.. optimization stops
4. Only one code at a time
5. *[find something for "no shirts no shoes"]*

A misnomered concept

There is no such thing as an “optimal code” tout court

Just try to give some example of what “optimal” is..

A misnomered concept

MEMORY CONSTRAINTS
memory imprint (of data and of the code itself)
possibly opt for repeating time-consuming ops

ENERGY CONSTRAINTS
Consuming as little energy as possible (or less)

I/O CONSTRAINTS
carefully crafting I/O (disk, memory, network,..)
don't forget reliability and resilience

"OPTIMIZATION"

TIME CONSTRAINTS
faster execution → shrink the time-to-solution
(worst case? optimal case? "average case"?)

ROBUSTNESS/RESILIENCE
You need a robust and resilient code at *mission-critical* level

A misnomered concept

MEMORY CONSTRAINTS
memory imprint (of data and of the code itself)
possibly opt for repeating time-consuming ops

ENERGY CONSTRAINTS
Consuming as little energy as possible (or less)

I/O CONSTRAINTS

"OPTIMIZATION"

Most of the time, you will have to cope with a variable combinations of ALL the previous factors.
And some additional ones, too.
(satellites' software is a good example)

(worst case? optimal case? average case ?)

resilient code at *mission-critical* level

A misnomered concept

Then, there is no such thing as an "optimal code" tout court

Probably you'd better think in terms of "*improved*" code.

- You don't want to hurt your code that honestly does its job: a faster code that gives incorrect ans. is not optimal in *any* way
- You most probably will have to re-use that code after some time. And you will need it to be *readable*.
- *Others* (sorry: **OTHERS**) most probably will have to read, understand and re-use that code.
- A clean, non-obscure, understandable, non-redundant code may not be "improved" in some way, but actually improves the quality of your life (and of the others' life).

So, why you may want to improve your code?

1) To have a **cleaner code**

2) To **re-design** (some of) its fundamental architecture (modules)

3) To **improve** the workflow, the memory imprint, the resource usage, the time-to-solution, …

A cleaner code | dryness

Be **DRY**: Don't Repeat Yourself

Duplication in logic → *abstraction* is the cure
Duplication in process → *automation* is the cure

Do neither add **unnecessary** code nor **duplicate** code

Unnecessary code increases the amount of needed work

- to maintain the code, either debugging or updating it
- to extend its functionalities

Duplicated code increases your *bad technical debt*, that already has a large enough number of sources:

- copy-and-paste programming style
- too much *agile* approach
- hard coding, quick-and-dirty fixes, cargo-cult, sloppiness

A cleaner code | readability

Readability is a pillar of **maintainability**.
Maintainability means that software can be extended, upgraded, debugged, fixed.

- **Baseline**: *write those damn comments*
- **Advanced**: *WRITE THOSE DAMN COMMENTS !*
  (possibly, use doxygen-like tools)
- **X-advanced**: avoid stupid, obvious, useless, confusing comments

Keep in mind: *"the code is the ultimate man page"*

A cleaner code | readability

- Use meaningful and coherent names and name modifiers inside functions and code blocks.
  Don't stick to the horrible `fortran`-like habit of unintelligible combinations of letters and digits: `var17u` doesn't mean nothing after few hours you wrote it. You have no more restrictions, and for sure you can find some more bytes in memory to put some useful name for variables and functions.
- Use meaningful and coherent conventions to name code blocks and to individuate the block a function belongs to.
- Clearly divide your code in different source files (that is unrelated to design: you may have a wonderful design awfully written in a unique 100k-lines source file).
- Adopt a coherent and consistent formatting: use in a logicla way indentation, blank lines, comment blocks, vertical spaces.

A cleaner code | readability

- Use m… …ions and co… Don't … …nations of letters… …wrote it. You ha… …ytes in memo…
- Use m… …o indivic…
- Clearly… …esign: you may h… …urce file).
- Adopt… …ntation, blank lines, comment blocks, vertical spaces.

Believe me.
You don't want me to get to your assignments and find some var or func name in that damn NR-style

```
QRV17_N
```

Or something else like

```
l = l + 1
This = that + O
```

No, you definitely don't want it.

A cleaner code, a cleaner programmer's life

1. Easier to understand even after months, or by someone else
2. Easier to catch side-effects of any changes
3. Easier to debug
4. Easier to find hot-spots
   - In memory footprints
   - In I/O and communications
   - In instruction intensity

Doesn't look like as "optimal" ?

So, why you may want to improve your code?

1) To have a cleaner code

2) To re-design its fundamental structure

3) To improve the workflow, the memory imprint, the resource usage, the time-to-solution

Re-design

If you want to re-design the whole code, you're probably writing a new code from scratch.

However, that is useful to stress a fundamental point:

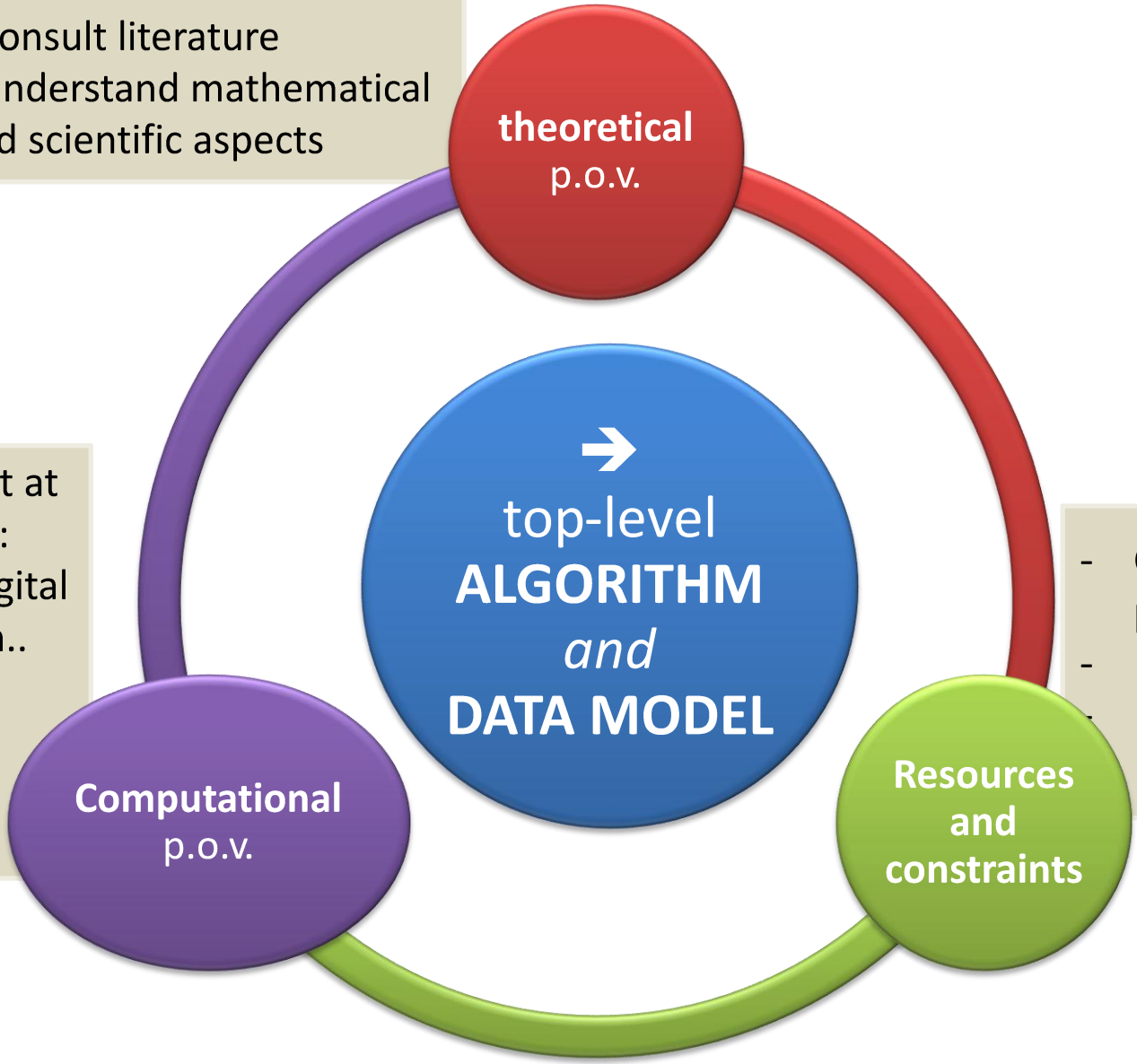
optimization starts from software's design

Sounds wonderful, isn't it? (a bit hipsteric, perhaps)

But: what is "design" ?

What is software design

- Consult literature
- Understand mathematical and scientific aspects

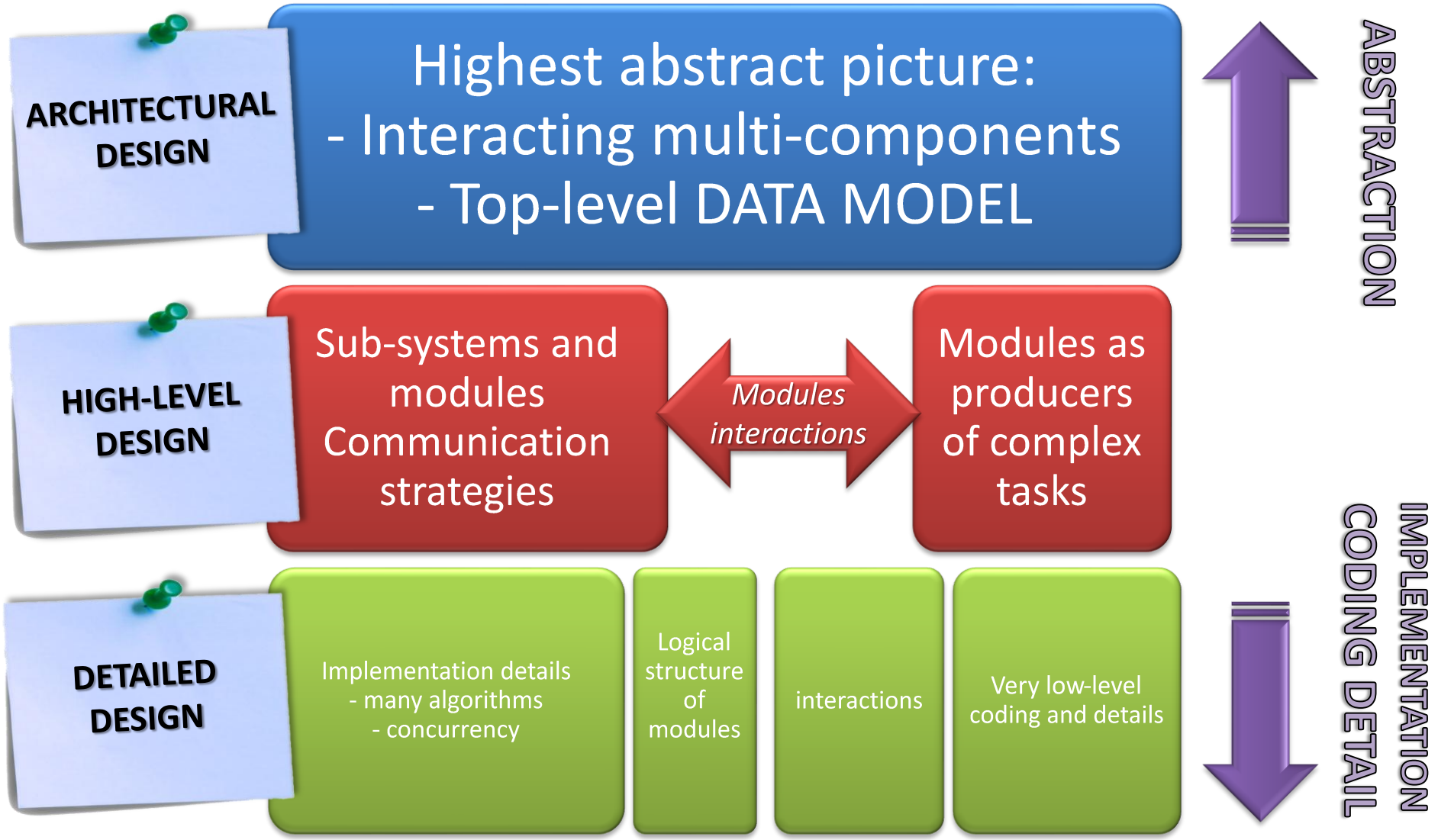


Well, you're not at the blackboard: you are on a digital discrete system..

(CFD is a good example of the concept)

- Concurrency/ parallelism
- Memory cnstr
- I/O cnstr
- Energy cnstr

What is software design



What is software design

MODULARIZATION

- On a functional basis, divide your problem in several coherent sub-problems of smaller complexity.
- Individuate relations among those sub-problems.
- Think in terms of **modules**, i.e. independent "objects" (or functions) able to independently carry on different tasks.
  - abstraction is easier
  - easier to maintain
  - re-usable
  - can be made concurrent
  - resiliency is enhanced

CONCURRENCY

Different modules (tasks) can run concurrently either on the same resources (CPUs/cores) or on different resources (cores / FPGA / GPUS / …).
They can be active at different times along the run.
They carry dependencies and conflicts with other modules (tasks).

What is software design

COHESION

The degree of intra-dependability **within elements of a module**.
The greater the cohesion, the better is the program design.

Logical cohesion - logically categorized elements are put together into a module.

Temporal Cohesion - elements organized such that they are processed at a similar point in time.

Procedural cohesion - elements grouped together, executed sequentially in order to perform a task.

Communicational cohesion – grouping of elements executed sequentially and working on same data

Sequential cohesion - elements executed sequentially taking outputs of previous one as inputs of following one.

Functional cohesion - Elements grouped because they all contribute to a single well-defined function. The highest degree of cohesion. Highly expected.

What is software design

COUPLING

The level of inter-dependability **among modules of a program**. It tells at what level the modules interfere and interact with each other.
The lower the coupling, the better the program (well… it depends).

Content coupling – a module can directly access or modify or refer to the content of another module.

Global/stamp coupling – multiple modules read and write to some global data (or different part of global structures).

Control coupling – a module decides the function of the another module or changes its flow of execution.

Data coupling – two modules interact with each other by means of passing data.

So, why you may want to improve your code?

1) To have a cleaner code

2) To re-design its fundamental structure

3) To **improve** the workflow, the memory imprint, the resource usage, the time-to-solution

…well, that is actually covered in Part II

Last steps in code design

TESTING IS part of the design 

- Unit test
  separately stress each unit of the code
- Integration test
  stress the integrated behavior of all the units together
- System test

VALIDATION and **VERIFICATION ARE** part of the design 

- Validation ensures that the code does what it was meant to do
  (all modules are designed accordingly to design specifications)
- Verification ensures that the codes does what it does *correctly*
  (black-box testing against test-cases, …)

Last steps in code design

TEST

- U
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- In
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- Sy

VALI

- Va
  (al
- Ve
  (black-box testing against test-cases, …)

Believe me.

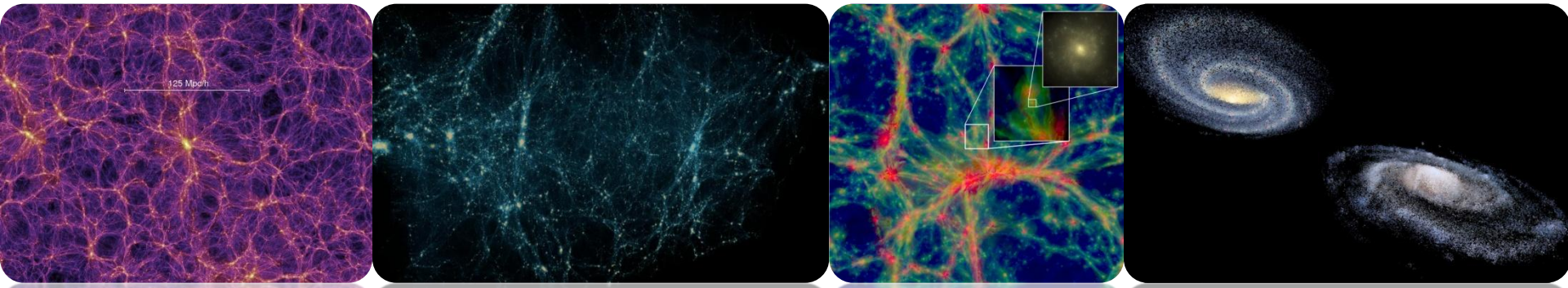
Neither, you don't want me to get to your assignments and find that you did not test a function or a module.

Or that you don't validate & verify your code after every change.

nt to do

orrectly

A sketched example: cosmological simulations



Simulation, in a cosmological framework, of the formation of

- The **cosmic structures** – LSS, galaxy clusters and galaxies.
- The **astrophysical processes** that drive their evolution and interactions.

With:

- **DM**, **DE** and **Baryons**.
- **Gravity** (long-range) + a **variety of interactions** at medium- and short-ranges.

A sketched example: cosmological simulations

Architecture
– highest level of abstraction –

Data Model

- arrays of structures vs structures of arrays
- what data are needed (← physics modules) / how to make it easy to add data (i.e. physics modules)
- some data (position, velocity, acceleration, ID, …) common among modules

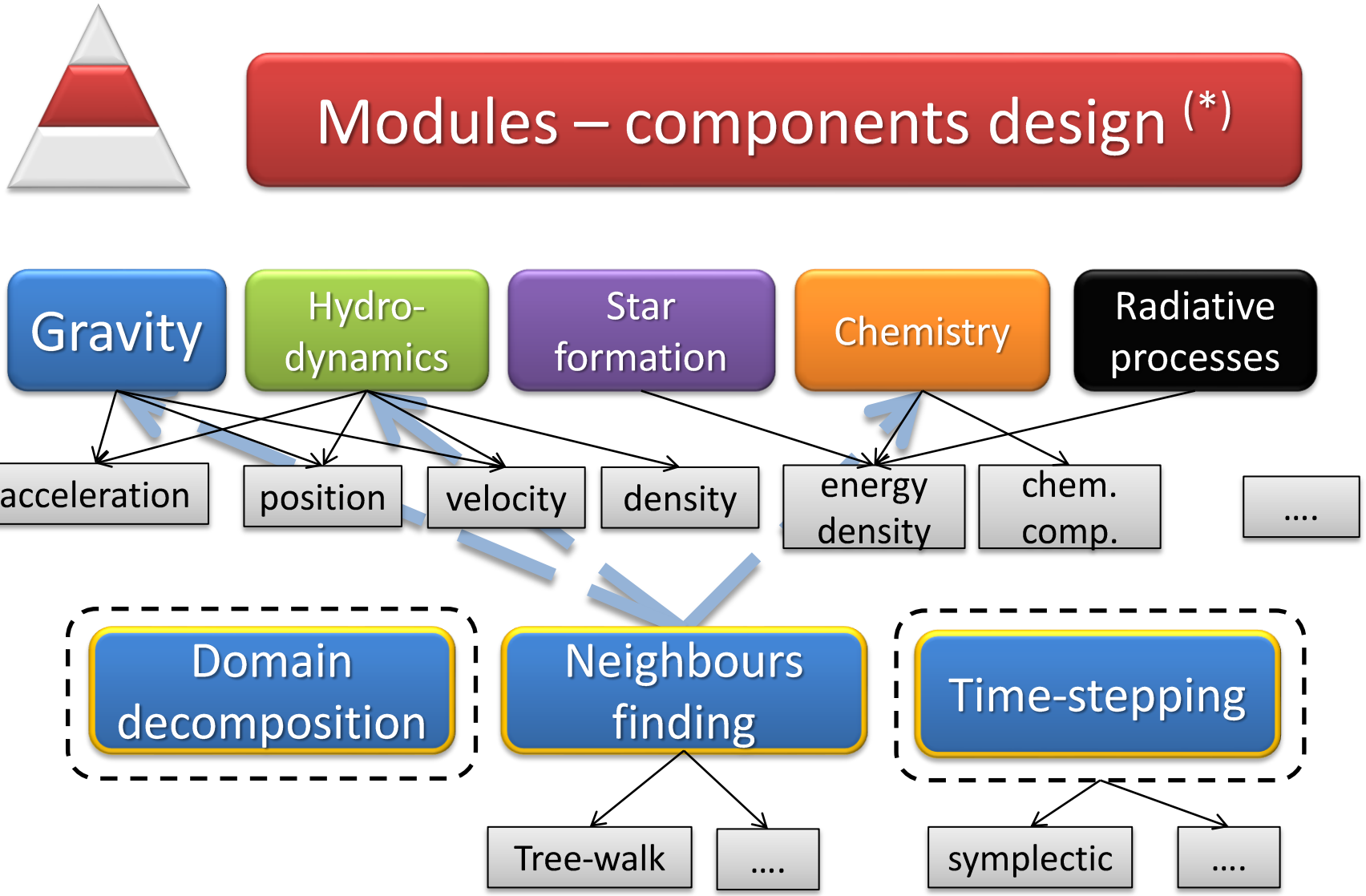
Execution

Massively Parallel is mandatory.
What paradigm? MPI, MPI+OpenMP/pThreads, PGAS, …

Concurrency

Task based, fine granularity ? ← easily to substitute physical modules
Rigidly procedural ?

A sketched example: cosmological simulations



(*) I should have used Data Flow Diagram, Structure Charts, UML, …

A sketched example: cosmological simulations

Implementation – Details

Gravity

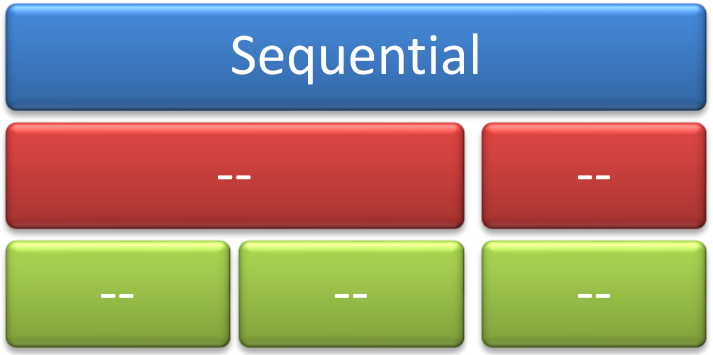
- Direct summation
- Pure PM
- TreePM
- Fast Multipole methods
- …

Hydro-dynamics

- Eulerian
  - multigrid
- SPH
- Mesh-free
- ….

…

- ….



Vs.