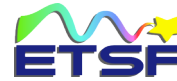


CECAM Lyon February 2008

## **Basic techniques and tools for the development and maintenance of atomic-scale software : the context**

X. Gonze  
Université Catholique de Louvain



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### **Who ? What ?**

Most lecturers & tutors : members of the Nanoquanta network  
and of the European Theoretical Spectroscopy Facility.

- Not computer scientists or professional developers.
- Still, experts in development and maintenance of softwares for atomic-scale simulation

=> This school : not a well structured set of software engineering lectures (would need university course), but a complement for high-level scientists who already develop software, and have no formal training in software engineering

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## The Nanoquanta 'Network of excellence'

Funded by the European Union (FP6) 1 June 2004 - 31 May 2008

10 nodes (over 100 researchers) : York (Godby), FHI Berlin (Scheffler), FU Berlin (Gross), Jena (Bechstedt), Louvain-la-neuve (Gonze), Lund (von Barth), Milano (Onida), Paris (Reining), Roma (Del Sole), San Sebastian (Rubio)

Scientific expertise : Ab initio simulations specialized on the interaction between matter and radiation (electrons, light, X-rays, lasers) and transport at the nanoscale

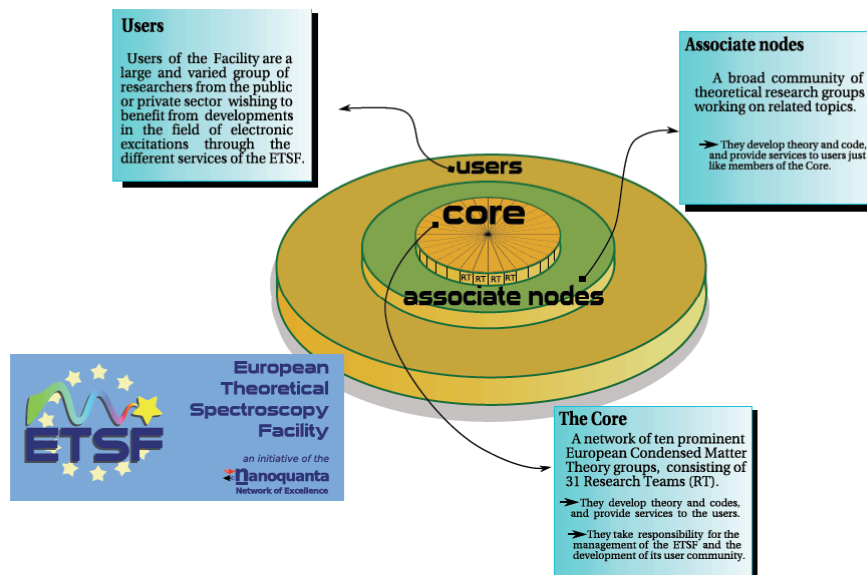
Goal : not really research, but integration ...

to launch the « European Theoretical Spectroscopy Facility »

(similarities / differences with the European Synchrotron Radiation Facility)

<http://www.nanoquanta.eu> and <http://www.etsf.eu>

## The European Theoretical Spectroscopy Facility



## The European Theoretical Spectroscopy Facility (II)

Pilot call for proposals March 2007 (more than 50 received proposals)

End of June 2007, approval by the EU (framework program 7) of the ETSF proposal for e-infrastructure :

- user's project
- software maintenance
- formation

Note : not a supercomputer center, but an expertise infrastructure, providing software, formation, support

## Integration of software (I)

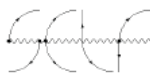
Many different software packages are used by the groups inside nanoquanta, including VASP, WIEN2K, SIESTA, QUANTUM-ESPRESSO, ...

Some softwares are developed or belongs to groups within Nanoquanta (NQ) :

- ABINIT
- FHI98PP (FHI Berlin) [www.fhi-berlin.mpg.de/th/fhi98md/fhi98PP](http://www.fhi-berlin.mpg.de/th/fhi98md/fhi98PP)
- DP (attached to Paris) [theory.polytechnique.fr/codes/dp](http://theory.polytechnique.fr/codes/dp)
- OCTOPUS (San Sebastian/FU Berlin) [www.tddft.org/programs/octopus](http://www.tddft.org/programs/octopus)
- EXC (Paris) [theory.polytechnique.fr/codes/exc](http://theory.polytechnique.fr/codes/exc)
- TOSCA (Milano)
- SELF (Roma / San Sebastian) <http://www.fisica.uniroma2.it/~self>

(especially strong for GW / TDDFT / Bethe-Salpether equation)

Funds were allocated to Integration Team 9 to hire Software Engineers for performing selected integration tasks.



## Integration of software (II)

Integration team 9 work :

- Recommendations for coding within NQ (good practices)
- File Format Specifications for Nanoquanta, based on the NetCDF library  
Crystallographic data files, wavefunction files, density/potential files,  
see <http://www.etsf.eu/fileformats>
- NQ library for XC functionals

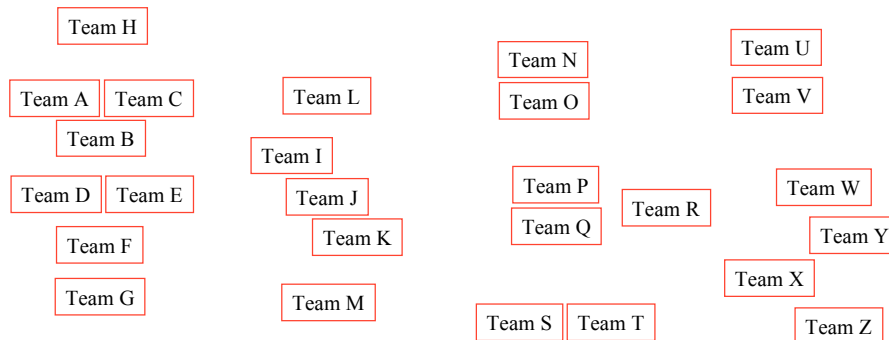
Software engineer projects :

- Packaging of all GPL softwares available within NQ  
(RPM/Debian ; live CD)
- Pseudopotential converter
- GUIs (one for OCTOPUS ; one for all Plane Wave based codes)
- creation of a library of F90 as well as C routines for reading/writing the  
NQ NetCDF files

## Relationships between developers (I)

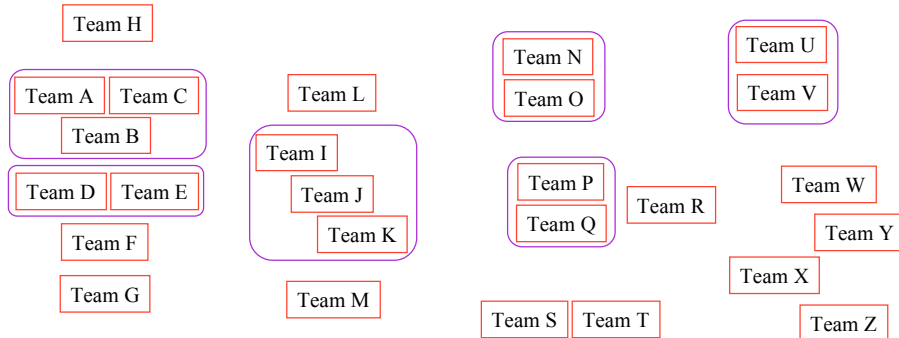
People located at the same place (a team)

*May be 20 developer teams currently in Europe for ETSF ?*



## Relationships between developers (II)

People located at the same place (a team)  
Different teams may contribute to the same project  
*E.g. : to develop GW in ABINIT*

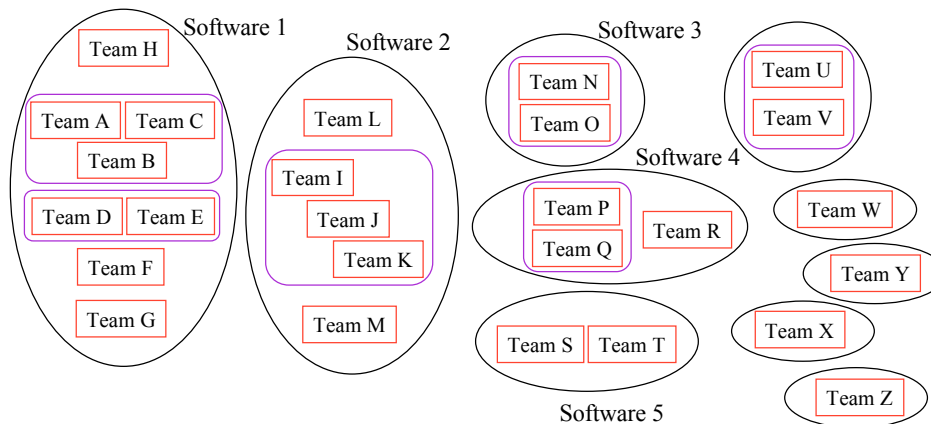


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## Relationships between developers (III)

People located at the same place (a team)  
Different teams may contribute to the same project  
A software benefits from several teams working on different projects  
*E.g. : ABINIT, CASTEP, CPMD, PWSCF, SIESTA, VASP, WIEN2K*



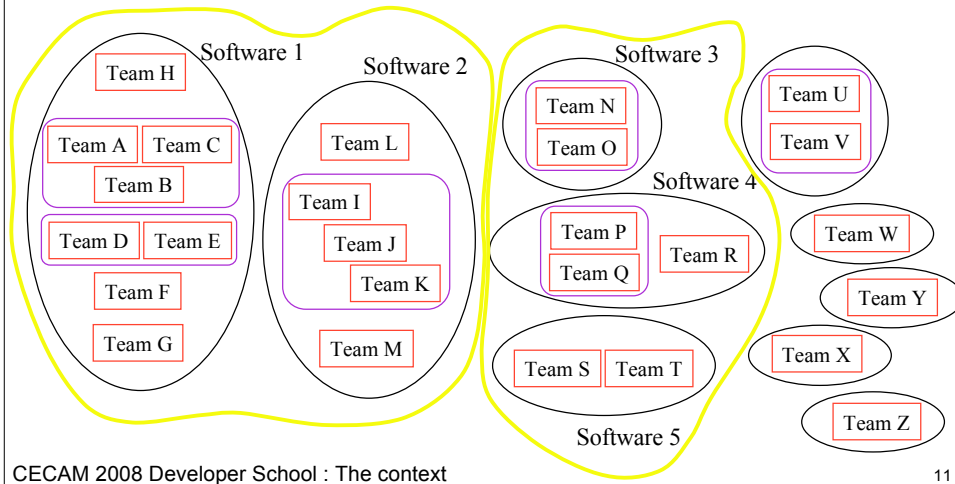
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## Relationships between developers (IV)

Different softwares can coordinate and be delivered in distributions.

*E.g. : Quantum-Espresso ; Nanoquanta/ETSF*

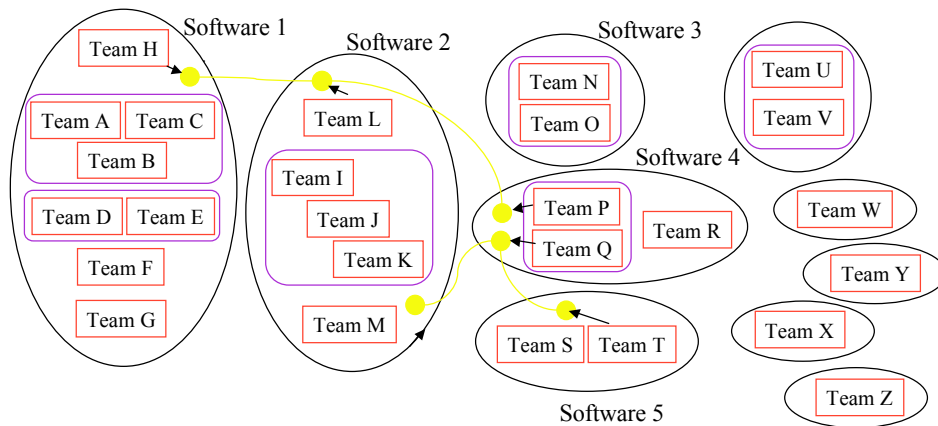


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## Relationships between developers (IV)

Software packages under a free licence can share free libraries

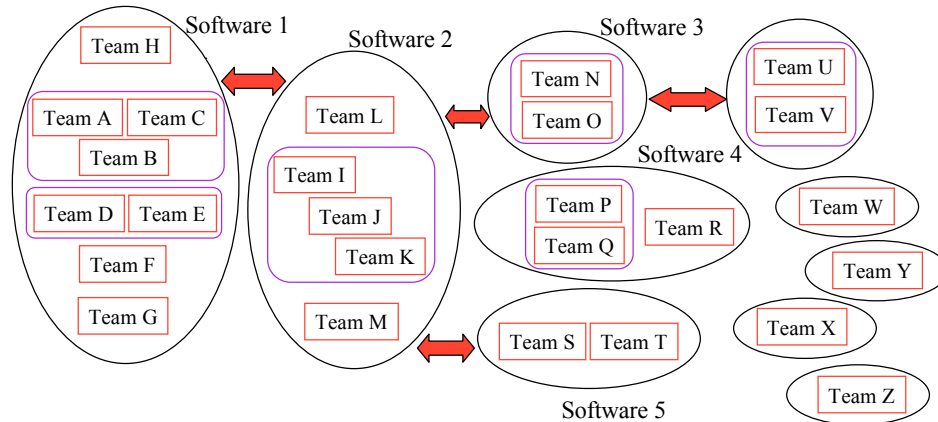


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## Relationships between developers (V)

Software packages can share common file formats, and exchange files



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## Goal of the tutorial

The goal of the tutorial will be to improve the ability of the participants to produce software that

- will have a long life cycle,
- is adequate for group software development,
- is re-usable,
- can better communicate with other atomic-scale software,
- executes correctly,
- is portable,
- possesses an acceptable execution speed.

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