Yambo: an ab-initio tool for excited-state calculations
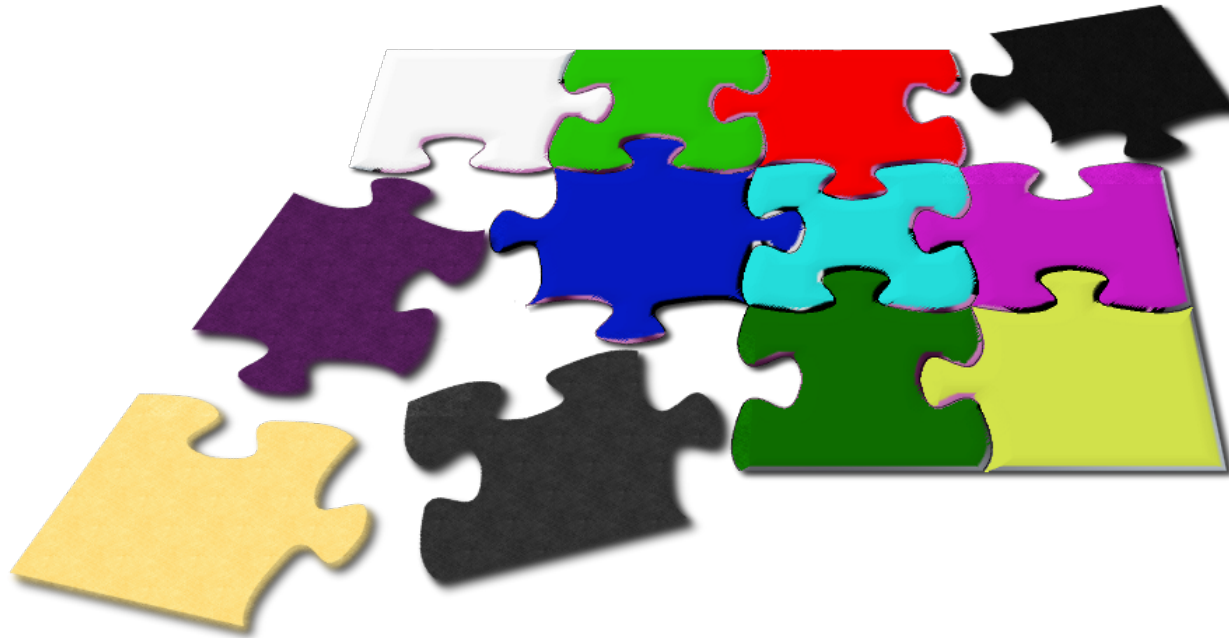
Yambo: combination of projects
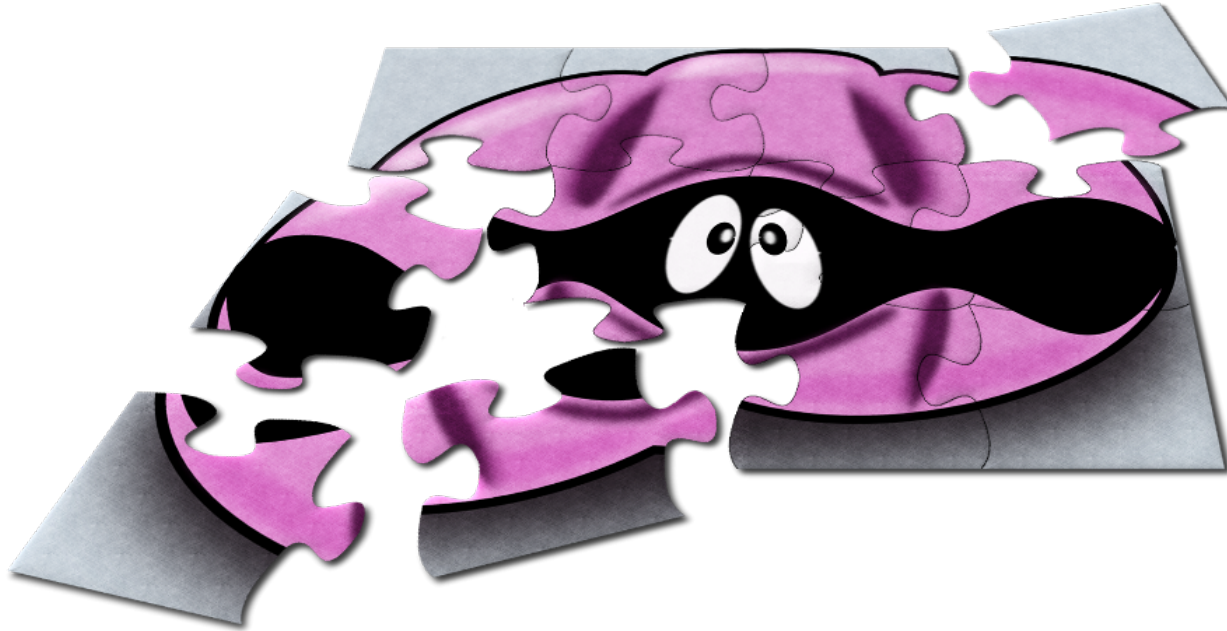
each developing a new numerical tool for
ab initio calculations of excited-state properties
of electronic systems

Yambo: one source many execs

mixed Fortran/C code:
core part + many extensions (part of them GPL)
Pieces of code stand-alone or joint together

Yambo: team of researchers

Conor Hogan Elena Cannuccia

Claudio Attaccalite

Andrea Marini

Davide Sangalli Daniele Varsano

Myrta Grüning

Working in different fields of
solid state physics
& molecular physics

Yambo from theory to applications:

Theory&approximations

Many-Body
Perturbation Theory

Time-dependent
density functional theory
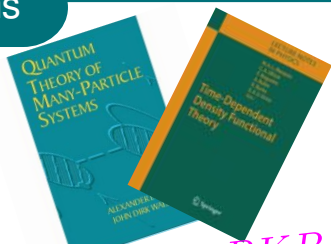
$$P = P_0 + PKP_0$$

Interfaces

Planewave
Pseudopotential codes

PWscf

abinit.org

$\{\psi_i^{KS}, \varepsilon_i^{KS}\}$
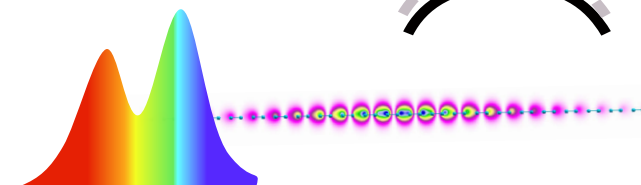
Performance

ScaLAPACK

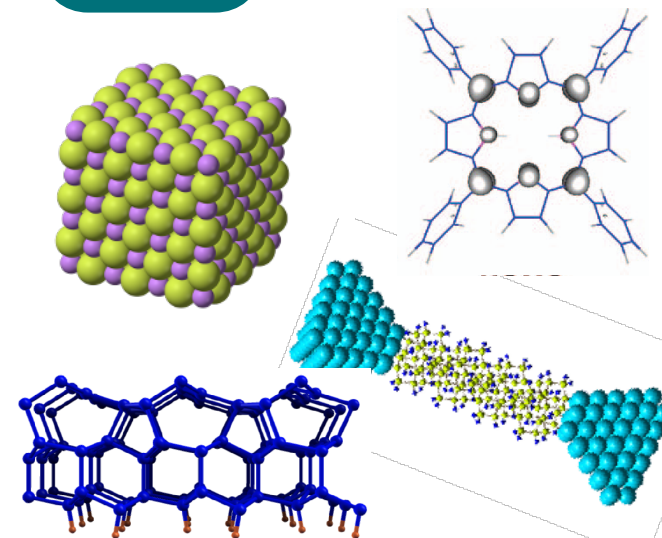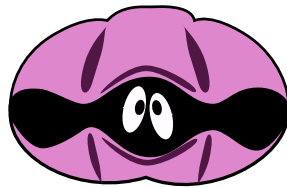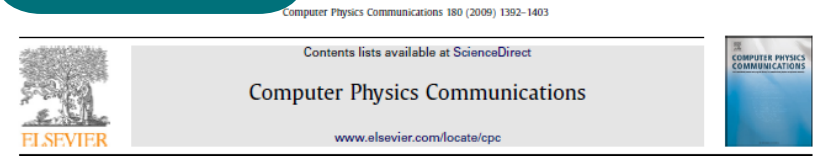MPI   FFTW   NetCDF

Properties

Quasiparticle (GW)

Excitons (BSE)

Plasmons...

Systems

Yambo researchers2researchers:

Main reference

Computer Physics Communications 180 (2009) 1392–1403

Contents lists available at ScienceDirect

Computer Physics Communications

www.elsevier.com/locate/cpc

yambo: An *ab initio* tool for excited state calculations ☆

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e European Theoretical Spectroscopy Facility (ETSF)
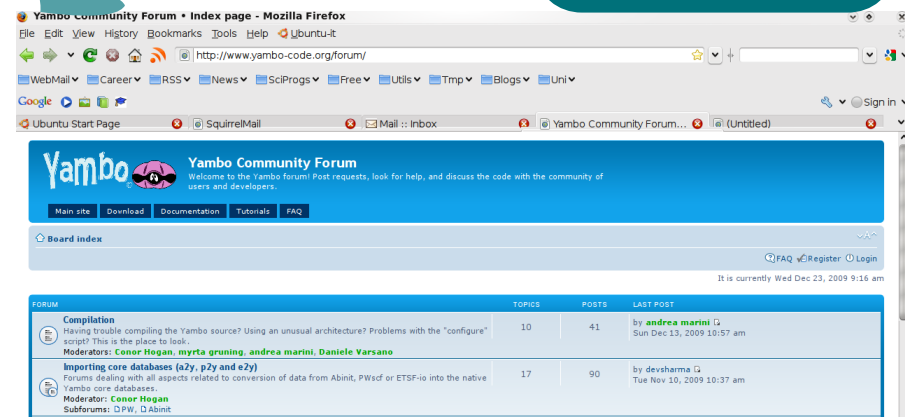
Comp. Phys. Comm. 180 (2009) 1392

Website

www.yambo-code.org

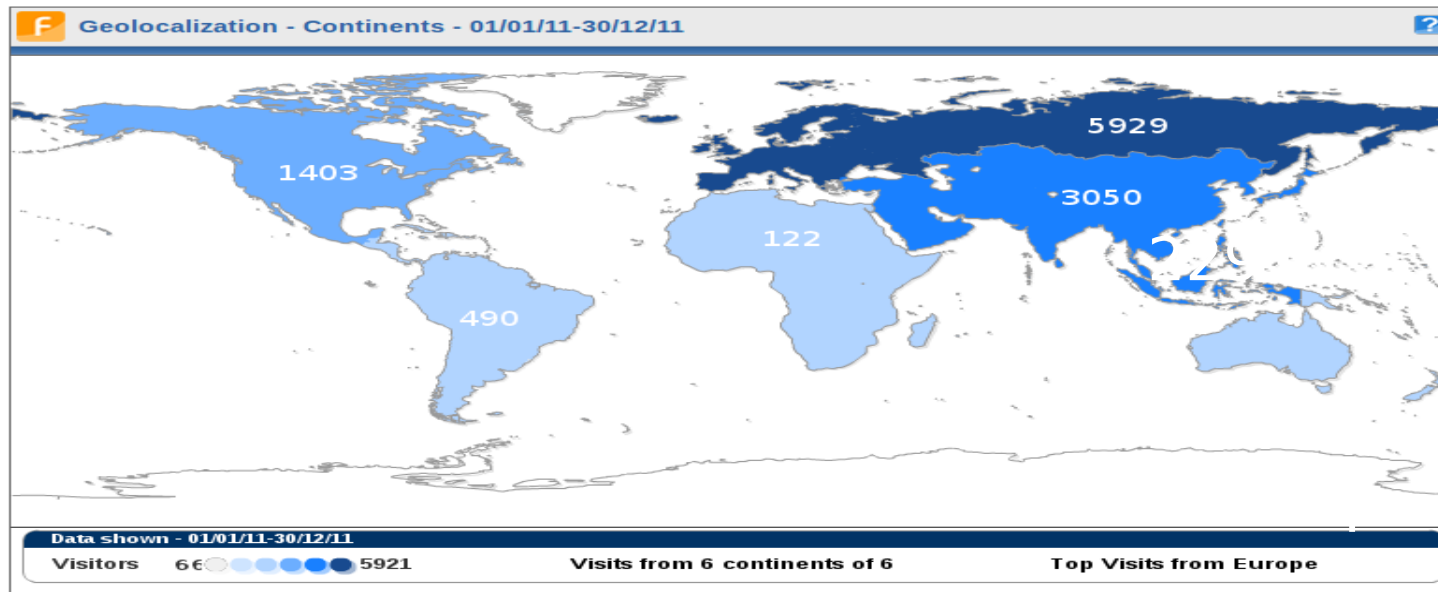news, infos, source, documentation, tutorials...

Community forum

www.yambo-code.org/forum

feedback, exchange and support

Yambo community of users

Geolocalization - Continents - 01/01/11-30/12/11

5929
1403
3050
122
490

Data shown - 01/01/11-30/12/11
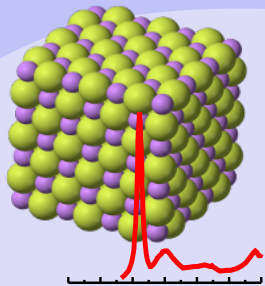Visitors 66○○○●●●● 5921   Visits from 6 continents of 6   Top Visits from Europe

2011: visits to the website

Yambo giant slalom:

Step by step introduction to Yambo (11/01)

Excitons in LiF (11/01):
comparison of theories & approximations

H-chains (12/01):
reasons for the ALDA failure