Computational Material Science: The Yambo perspective
Yambo in the Materials Science World

Yambo: (super) short introduction

Yambo: from theories to GPU’s

The Yambo Philosophy
Actors in Material Science

Experimentalists (Motto: Theoreticians do not understand what we measure)

Theoreticians (Motto: Experimentalists do not understand what they measure)

Runners (Motto: If it exists we can simulate it!)

Technical sheet

Model: IBM BlueGene/Q
Architecture: 160Q Frame with 2 MidPlanes each
Front-end Nodes: OS: Red Hat EL 6.2
Compute Node Kernel: lightweight Linux-like kernel
Processor Type: IBM Power62, 1.6 GHz
Computing Nodes: 10,240 with 16 cores each
Computing Cores: 163,840
RAM: 16GB/node, 1GB/core
Internal Network: Network Interface with 11 links --5D Torus
Disk Space: more than 2PB of scratch space
Peak Performance: 2.1 PFlops
Theoretical Physics
\[ H = \sum_i h(x_i, p_i) + \frac{1}{2} \sum_{i \neq j} \left| x_i - x_j \right|^{-1} \]

\[ H \approx \sum_i h(x_i) \]
**DFT**

- Fully interacting system
  - Hohenberg-Kohn Theorem
  - Same Ground-State density $n(r)$

- Non interacting system
  - Kohn-Sham particle

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**MBPT**

- Fully interacting system
  - Diagrammatic Expansion
  - Same Excitation Spectra

- Weakly interacting system
  - $\bullet$ particle

- Weakly interacting system
  - $\circ$ hole

---

- Weakly interacting system
  - $\bullet$ particle
  - $\circ$ hole
  - $\cdots$ $W$
The AiMBPT (Ab-Initio Many-Body Perturbation Theory) is parameter free, predictive, accurate, and universal. It is based on DFT (Density Functional Theory) and MBPT (Many-Body Perturbation Theory). The AiMBPT is given by:

\[ G(r_1, r_2; t) \propto \langle \psi(r_1, t) | [\psi^+(r_2)) \rangle \]

where \( \psi(r) \) is the wave function, \( V(r) \) is the potential, and \( V_{\text{Hxc}}(r) \) is the exchange-correlation potential. The AiMBPT is used to calculate the ground state energy and properties of materials. The AiMBPT is a powerful tool for predicting the properties of complex systems.
The Ab-Initio "Way":
Codes & Physics...

Adapted from M. van Schilfgaarde et al. PRL 96 (2006)
Theoretical Physics
Yambo?!?! No!! SELF (2000)

The Origin of the Theses

if (outcome != bad && 😊 == fun) {
    thenWhyNot();
}
Many-body perturbation theory calculations using the Yambo code,
Theory
MBPT, DFT, TDDFT, NEGF

Interfaces
Planewave Pseudopotential codes:
abinit.org
PWscf

Libraries
ScaLAPACK
ioth
libxc
FFTW
netCDF
ETSF-io
MPI2

Different projects

Developers
www.yambo-code.org

the Yambo team
Provides an introduction to Yambo-GPL, detailing its applications and properties.

**Properties**
- GPL
- Quasi-particles
- Optical absorption
- Electron energy loss
- Magneto optical properties
- Electron-phonon coupling
- Surface spectroscopy

**DEVELOPMENT / PRE-GPL**
- Out of equilibrium dynamics
- Multi-level parallelization

**Applications**
- Image of a complex structure
- Image of a material property
- Image of a simulation output

**Schools**
- Screenshot of an educational resource

**Community & Publications**
- Growing community of users using Yambo for forefront research.
- More than 200 publications.

**Support & reach out**
- Git repository

**Dedicated User Forum**
- Screenshot of a forum discussion

**Online documentation and tutorials**
- Screenshot of a tutorial page

**www.yambo-code.org**
International Communicative Collaborative Performance Communicative Collaborative
Be collaborative
Dissemination

Main Page

Welcome to the Yambo educational page. In this page you will find several informations about how to run Yambo and, more generally, about the methods implemented in the code.

Contents [hide]
1. Yambo Philosophy
2. Read
3. Learn
4. Run
5. Close

Yambo
Educational

Computational School on Electronic Excitations in Novel Materials
the Yambo Code

27 - 31 January 2020
Trieste, Italy

1st CENTRAL AFRICAN SCHOOL ON ELECTRONIC
STRUCTURE METHODS AND APPLICATIONS (CASESMA)
NOVEMBER 18 - 23, 2019 DACHANG, CAMEROON

With the financial support of The Abdus Salam International Centre for Theoretical Physics (ICTP), Italy, the African School on Electronic Structure Methods and Applications (ASESMA) in collaboration with the University of Dachang, is organizing the “1st Central African School on Electronic Structure Methods and Applications (CASESMA)” to be held from November 18 to 23, 2019 in Dachang, Cameroon.

OBJECTIVES
With the increasing power and affordability of computers, electronic structure methods will be shown as a powerful tool to address challenging problems in physics, chemistry and materials science and as a valuable alternative to circumvent the high costs of experimental equipments, which in most of the cases is not affordable in developing countries like Cameroon. The scientific program will focus on ab initio molecular dynamics and many body perturbation theory.

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Ibrahim Adetunji (Nigeria)
Anne Etindele (Cameroon)

APPLICATIONS
Theoretical Physics
\[
\left[ -\nabla^2 + v_{DFT}(r) \right] \psi_{nk}(r) = \epsilon_{nk} \psi_{nk}(r)
\]
Performance = CPU's & GPU's

MPI

OpenMP

FTTW

NetCDF

ScaLAPACK

PETSc

theYambo team
A “real life” example

- Yambo single GW calculation scaling up to 1000 KNL nodes (~ 3 PFI/s)
- hybrid MPI+OpenMP + scaLapack
- Calculations relevant for an active research field (graphene nanoribbons)
- Performed on a brand new architecture (Intel KNL @ Marconi)
Yambo on CPU...

**MPI**

- Dipoles
- X₀
- X
- Self energy
- Other

![Graph showing time performance vs. #MPI tasks and #Threads]

**OpenMP**

- Dipoles
- X₀
- X
- Sigma
- Other

![Graph showing time performance vs. #Threads]
Yambo on GPU...

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<td>Marconi-A2</td>
<td>Intel Xeon Phi7250 KNL</td>
<td>1.4</td>
<td>68</td>
<td>–</td>
<td>~ 3000</td>
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Table 6: Different computer architectures used to benchmark YAMBO.

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<tr>
<th>Architecture</th>
<th>Dipoles</th>
<th>$\chi^0$</th>
<th>$\chi$</th>
<th>$\Sigma_x$</th>
<th>$\Sigma_c$</th>
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<td>MARCONI-KNL</td>
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<td>16631</td>
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<td>Piz Daint CPU+GPU</td>
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<tr>
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<td>993</td>
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<td>35</td>
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<td>1639</td>
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</table>

Complete GW workflow for a N7 Graphene Nanoribbon Porting on NVIDIA GPUs done using CUDA Fortran + CUDA Libs
European codes in Material Science

- Chemical Sciences and Materials: 26%
- Fundamental Constituents of Matter: 18%
- Earth Sciences: 7%
- Maths and Comp. Sciences: 4%
- Engineering: 16%
- Others: 18%
- Electronic structure codes: 82%
- Quantum ESPRESSO: 34%
- YAMBO: 8%
- CP2K: 4%
- SIESTA: 4%
Yambo: the path from mistery to mastery
To go from mystery to mastery one has to:

- understand levels of complexity
- read & study theory
- learn through hands-on tutorials
What is behind 'running a simulation'?

Physical phenomenon

Theory & methods

Numerical implementation

Simulation
What is behind 'running a simulation'?

1. Physical phenomenon
2. Simplifying assumptions
3. Theory & methods
4. Discretization
5. Numerical implementation
6. Choice of parameters
7. Simulation

The Yambo team
How can we answer the following questions...

- accuracy?
- computational cost?
- applicability?

simplifying assumptions

physical phenomenon

theory & methods

choice of parameters

numerical implementation

discretization

simulation
The first step is to 'read & study':

- physical phenomenon
- light-matter interaction
- spectroscopy

theory & methods

numerical implementation

simulation
The first step is to 'read & study':

- density-functional
- linear response
- many-body

physical phenomenon

theory & methods

numerical implementation

simulation

the Yambo team
The first step is to 'read & study':

- discretised eqs.
- numerical methods
The second step is to 'learn' through hands-on tutorials: which methods for what phenomenon.
The second step is to 'learn' through hands-on tutorials:

- Physical phenomenon
- Theory & methods
- Numerical implementation
- Parameters choice for accuracy & computational cost
- Simulation

The Yambo Team
This school:

Choice of parameters? Applicability? Accuracy? Computational cost?

Hands-on tutorial

Lectures

Light matter interaction experiments
DFT, Linear response, MPBT
Bound Excitons in Time-Dependent Density-Functional Theory:  
Optical and Energy-Loss Spectra

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Via della Ricerca Scientifica, I-00133 Roma, Italy  
(Received 17 July 2003; published 16 December 2003)
1. Many-body perturbation theory calculations using the yambo code
2. Yambo: an ab initio tool for excited state calculations