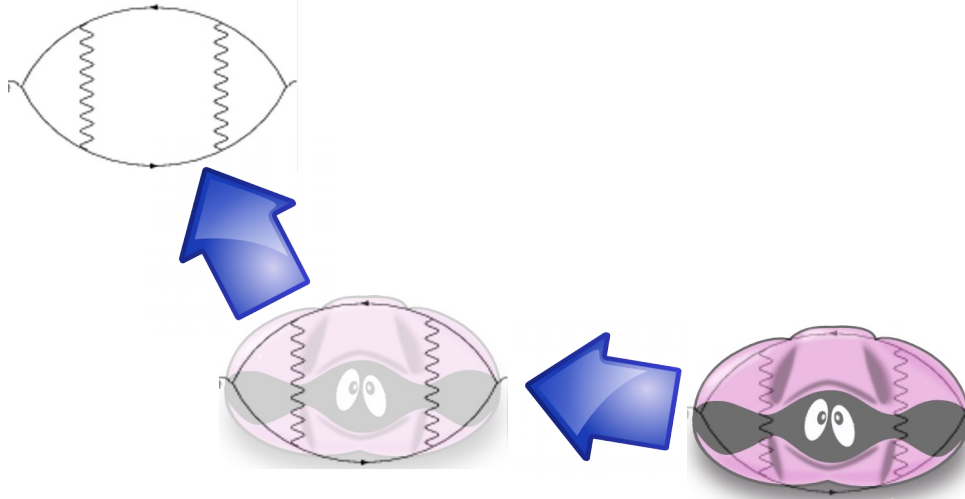




DRIVING
THE EXASCALE
TRANSITION



Computational Material Science: The Yambo perspective



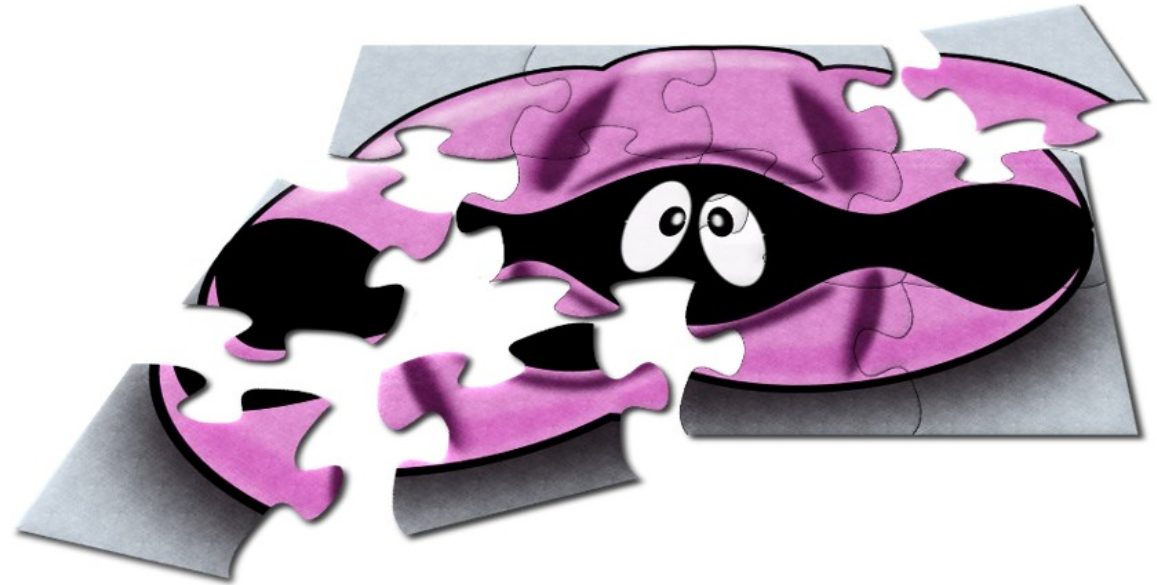
Outline

Yambo in the Materials Science World

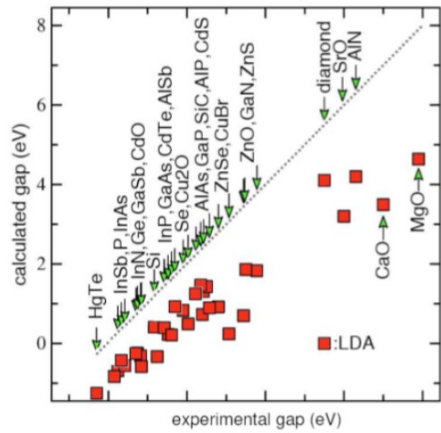
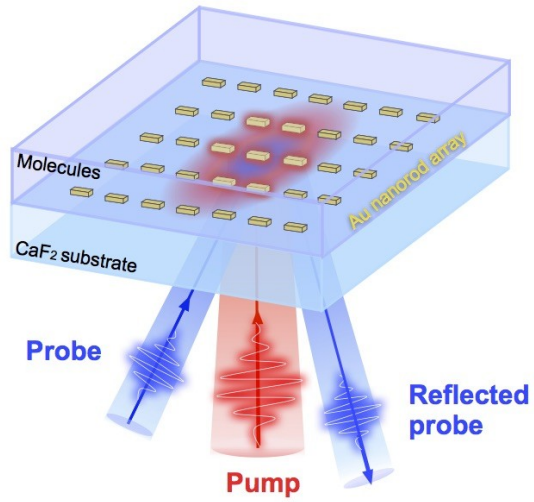
Yambo: (super) short introduction

Yambo: from theories to GPU's

The Yambo Philosophy

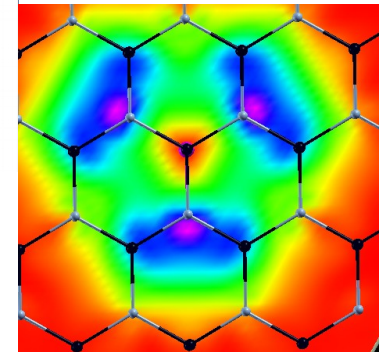
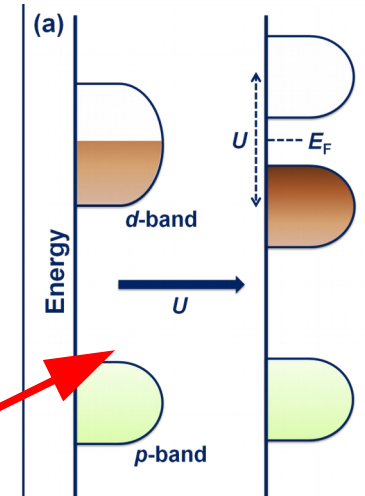
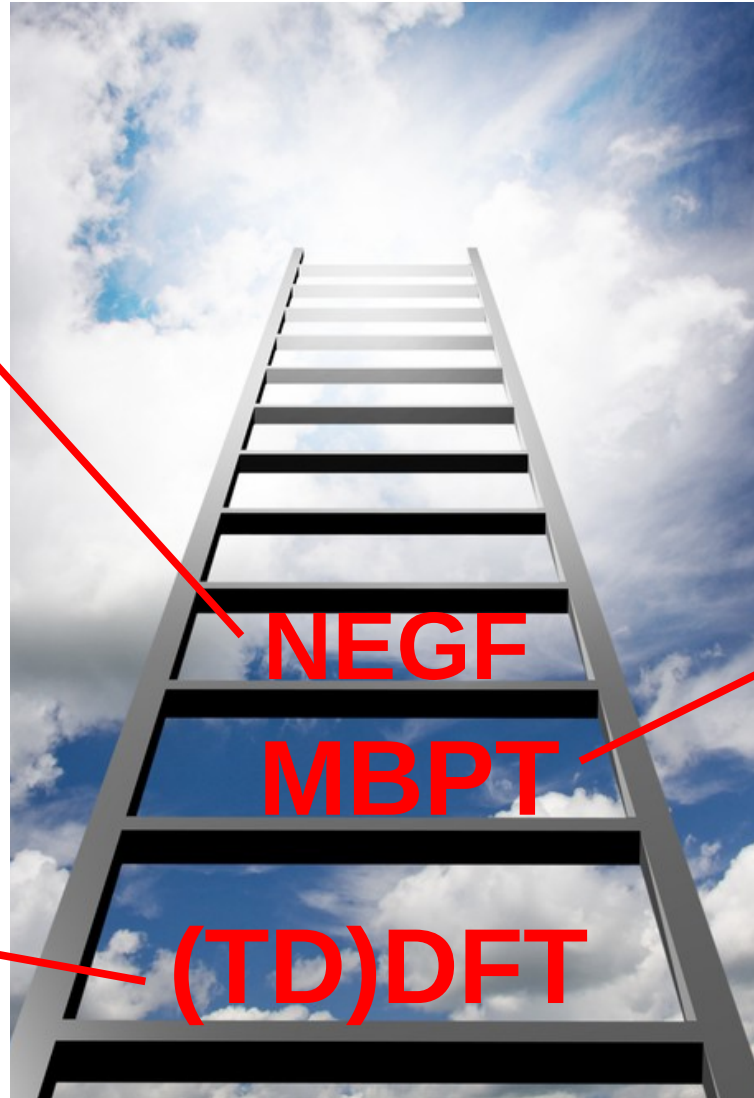


Theoretical Physics? Which one?



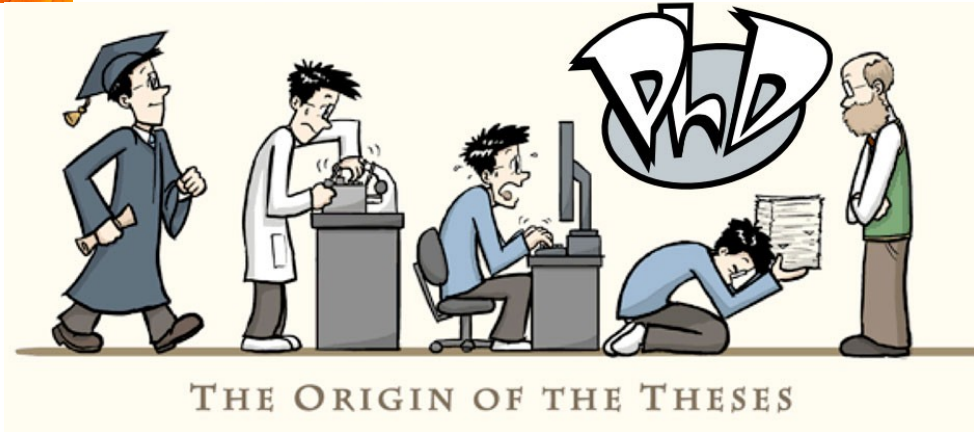
Si:
0.47 eV (LDA) vs 1.1 eV (expt)

GaAs:
0.30 eV (LDA) vs 1.4 eV (expt)

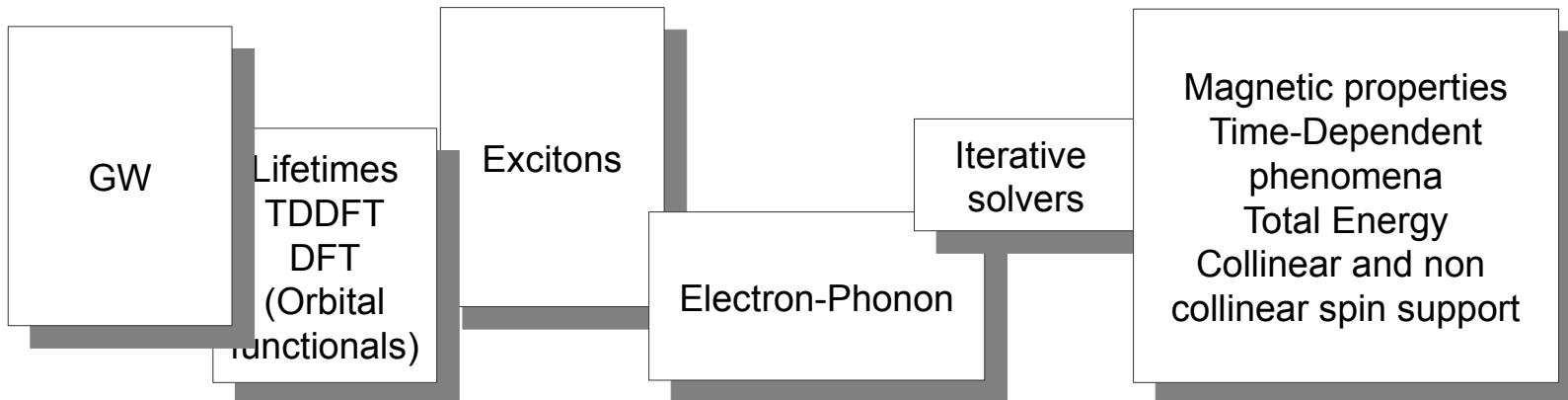
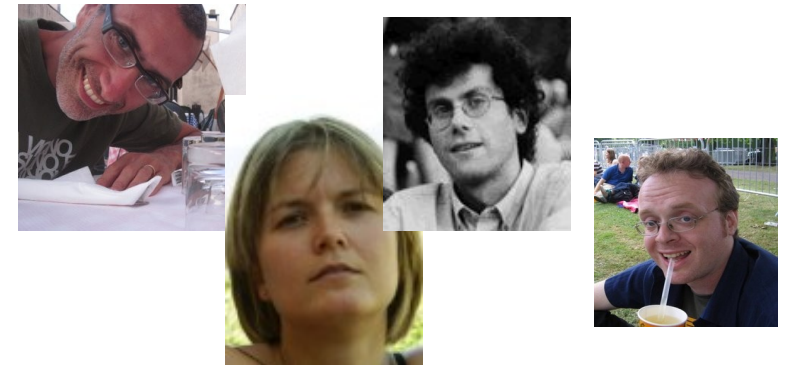


Adapted from M. van Schilfgaarde *et al.* PRL **96** (2006)

Yambo (yesterday)



Yambo: an ab initio tool for excited state calculations,
 A. Marini, C. Hogan, M. Grüning, D. Varsano,
 Comp. Phys. Comm. 180, 1392 (2009).



Yambo (today)

Yambo: an ab initio tool for excited state calculations

[A Marini](#), [C Hogan](#), [M Grüning](#), [D Varsano](#) - *Computer Physics ...*, 2009 - Elsevier

Abstract yambo is an ab initio code for calculating quasiparticle energies and optical properties of electronic systems within the framework of many-body perturbation theory and time-dependent density functional theory. Quasiparticle energies are calculated within the ...

☆ Cited by 679 Related articles ACNP Holdings

Many-body perturbation theory calculations using the Yambo code,
D. Sangalli, A. Ferretti, H. Miranda, C. Attaccalite, I. Marri, E. Cannuccia, P. Melo, M. Marsili, F. Paleari, A. Marrazzo, G. Prandini, P. Bonfà, M. O. Atambo, F. Affinito, M. Palummo, A. Molina-Sánchez, C. Hogan, M. Grüning, D. Varsano, A. Marini;
J. Phys.: Condens. Matter 32, 325902 (2019)

Yambo is a FORTRAN/C code for Many-Body calculations in solid state and molecular physics.

> 50 development branches!

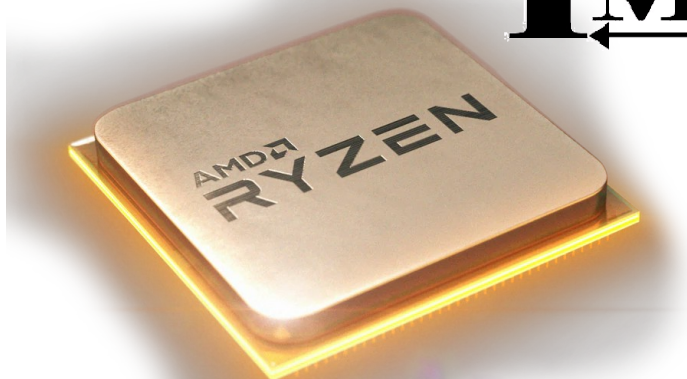
Forum, Wiki, Tutorials, Schools

Performance!

 ANDREA MARINI	 DANIELE VARSANO	 MYRTA GRÜNING	 CONOR HOGAN
 ALEJANDRO MOLINA-SANCHEZ	 MAURIZIA PALUMMO	 ANDREA FERRETTI	 DAVIDE SANGALLI
 CLAUDIO ATTACCALITE	 ELENA CANNUCCIA	 IVAN MARRI	 HENRIQUE MIRANDA
 MICHAEL ONTITA ATAMBO	 FABIO AFFINITO	 FULVIO PALEARI	 MARGHERITA MARSILI
 ANTIMO MARRAZZO	 PEDRO MELO	 GIANLUCA PRANDINI	 PIETRO BONFA

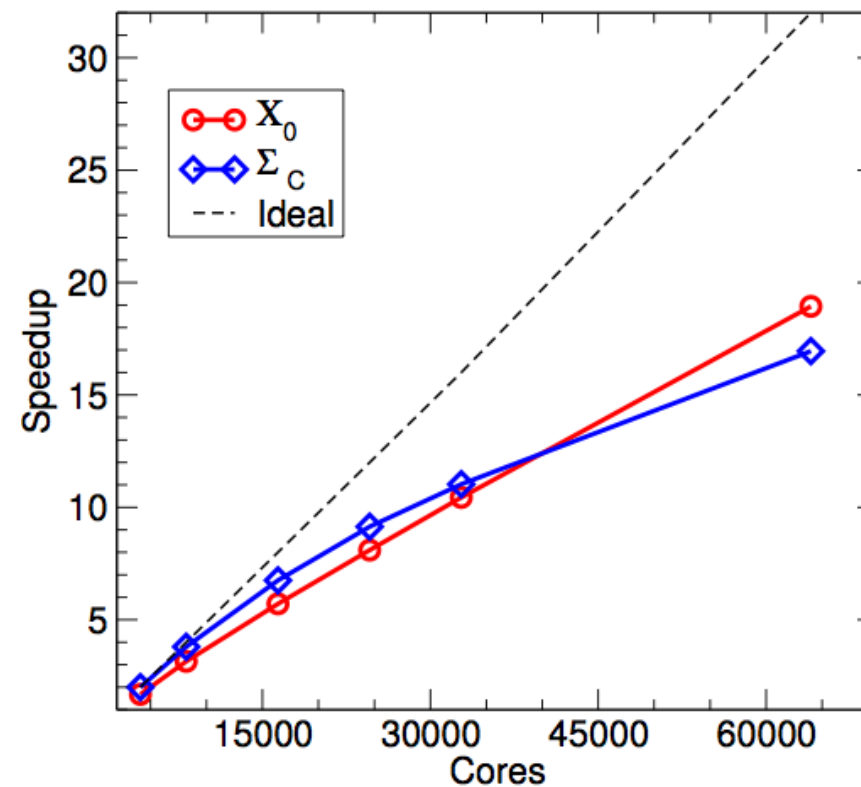
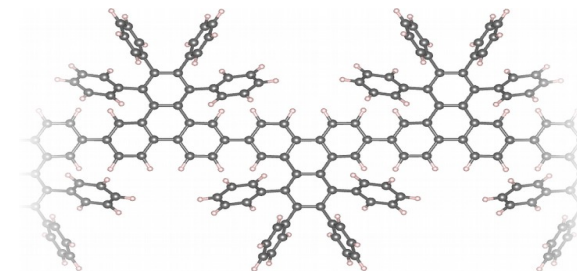
Performance on CPU and GPU

IMPI

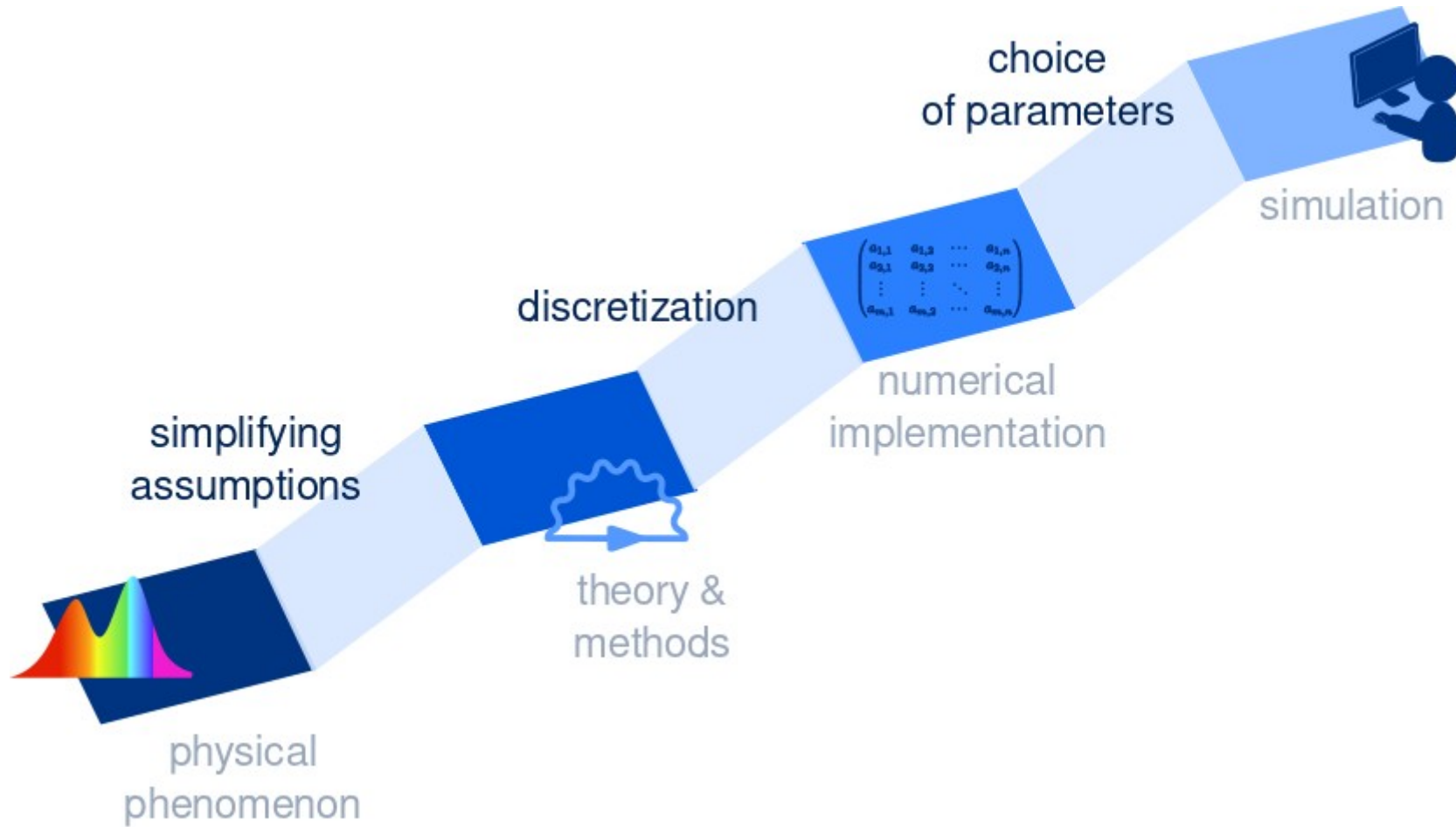


OpenMP

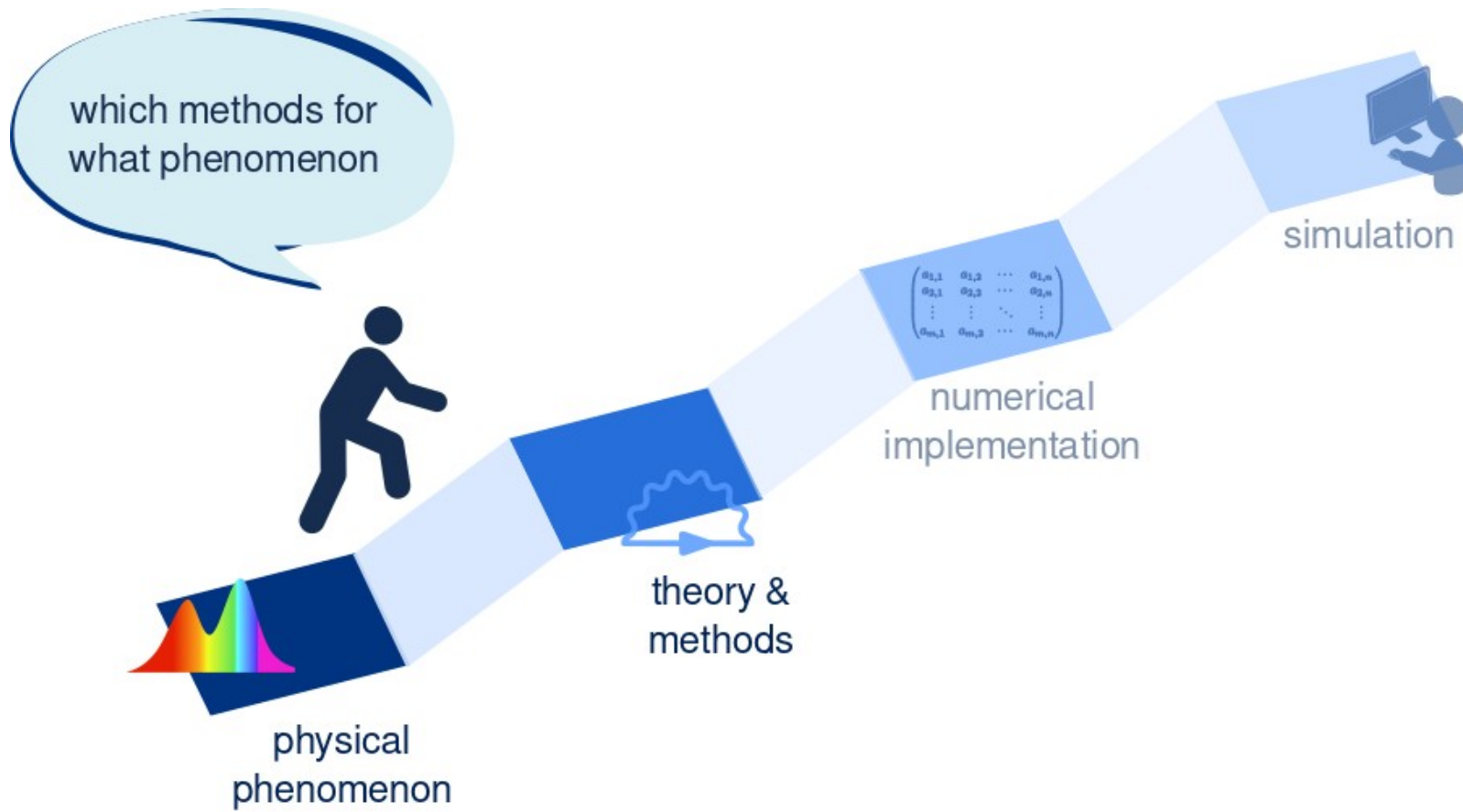
CUDA
FORTRAN



From the problem to the solution (I)



Step #1: LEARN by studying!



- Edu Home
- WWW Home
- Tutorials
- download
- Install
- Yambo Virtual Machine
- Developers Corner

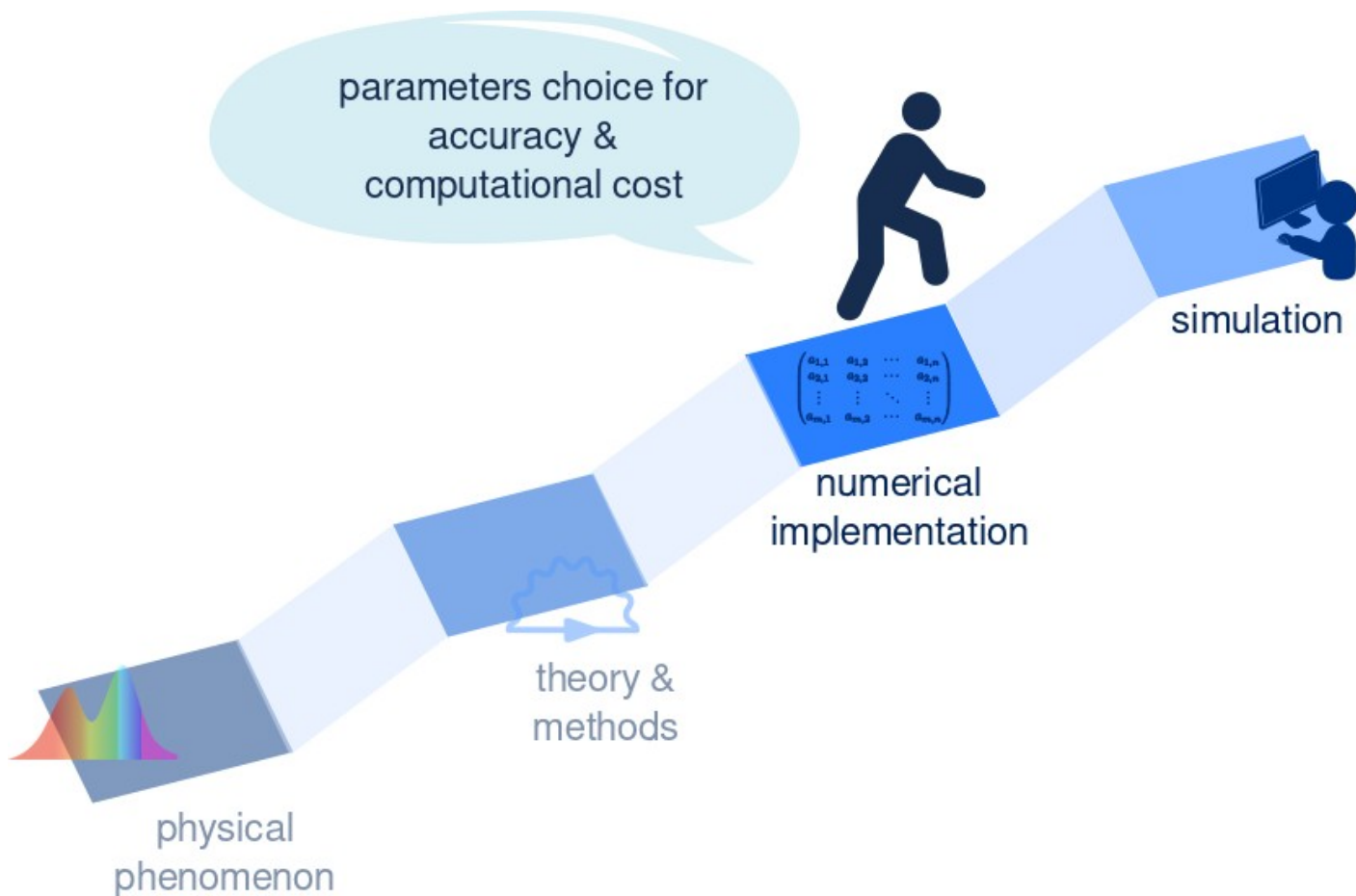
Page [Discussion](#)

Selected Readings

Contents [hide]

- 1 General Theory
- 2 Many-body Theory
- 3 The GW method
- 4 Density Functional Theory
- 5 TDDFT
- 6 Non-equilibrium Green's function
- 7 Theoretical Spectroscopy
- 8 Computer Programming

Step #2: LEARN by practicing!



Edu Home
WWW Home
Tutorials
download
Install
Yambo Virtual Machine
Developers Corner

Read!
Theory
Lectures
Cheatsheets
Selected Readings
Thesis

Learn! (Modular Tutorials)
Overview
First steps
GW basics
GW in parallel
GW convergence
BSE basics
BSE convergence
BSE for 2D
Exciton plots
Yambopy
All Modules

Page Discussion

Tutorials

Two kinds of tutorials are provided: **stand-alone** and **modular**.

Contents [hide]

- 1 Tutorial files
 - 1.1 Tutorial Repository (advanced users)
 - 1.2 Direct Download (all users)
 - 1.2.1 Files needed for modular tutorials
 - 1.2.2 Files needed for stand-alone tutorials
- 2 Stand-alone tutorials
 - 2.1 Basic
 - 2.2 Advanced
- 3 Modular tutorials
 - 3.1 Introduction
 - 3.2 Quasiparticles in the GW approximation
 - 3.3 Using Yambo in Parallel
 - 3.4 Excitons and the Bethe-Salpeter Equation
 - 3.5 Yambo-python driver
 - 3.6 Modules

Step #3: Ask Help!







Yambo Community Forum

Welcome to the Yambo forum! Post requests, look for help, and discuss the code with the community of users and developers.

FAQ

Board index

It is currently Wed Jun 10, 2020 2:08 pm

	SUBFORUMS	STATISTICS	LAST POST
	Compilation Having trouble compiling the Yambo source? Using an unusual architecture? Problems with the "configure" script? This is the place to look. Moderators: Davide Sangalli , Daniele Varsano , andrea.ferretti , andrea marini , myrta gruning , Conor Hogan	Topics: 154 Posts: 1039	Re: Compilation error of Yamb... by palfu  Mon Jun 08, 2020 1:06 pm
	Importing core databases (a2y, p2y and e2y) Forums dealing with all aspects related to conversion of data from Abinit, PWscf or ETSF-io into the native Yambo core databases. Moderators: andrea.ferretti , Conor Hogan Subforums: PW , Abinit	Topics: 75 Posts: 397	Re: qe 6.5 and yambo 4.5: fmt... by chwolf  Wed May 06, 2020 6:13 am
	Running Yambo Yambo can be operated on several different runlevels: here you will find several forums that deal with the specific physical task that you are trying to carry out. Subforums: Initialization , Linear Response , Self Energy , Other issues , Spin dependent and spinorial calculations , Electron Phonon effects	Topics: 769 Posts: 4401	initialization for ELPH datab... by ymzhang 



DRIVING THE EXASCALE TRANSITION

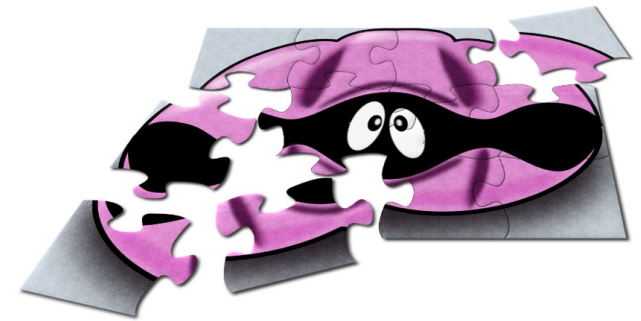
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THANKS



<http://www.yambo-code.org/>