Introduction to the Ab-Initio Many-Body Perturbation theory: codes and applications

Andrea Marini

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FLASH it

www.yambo-code.eu

Istituto di Struttura della Materia

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http://www.yambo-code.eu/andrea

The Materials Science World

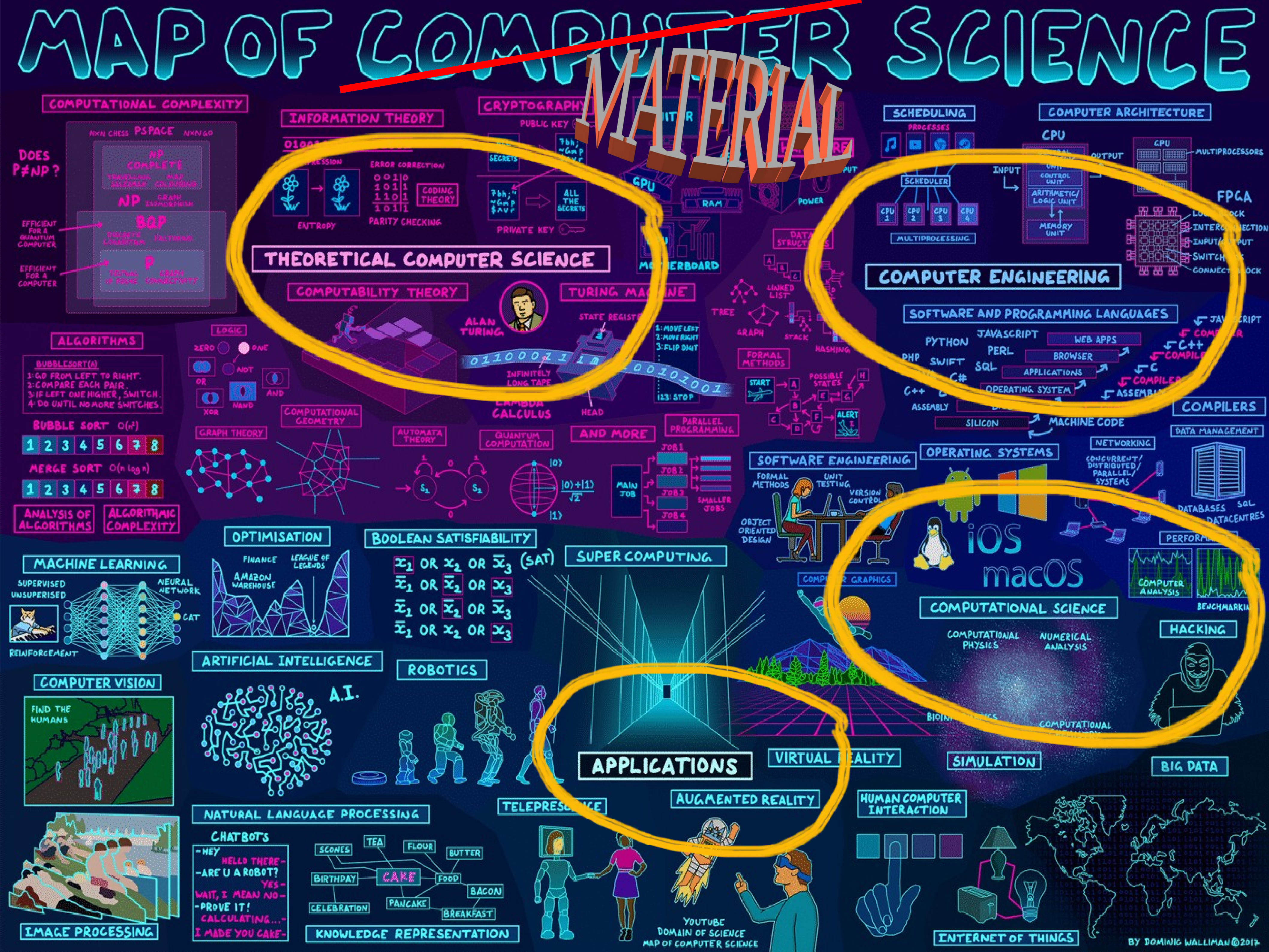
Many-Body Perturbation Theory for dummies

Yambo: from theories to GPU's

The scientific Method

the Yambo team

The Materials Science World



MAP OF COMPUTER SCIENCE
MATERIAL
COMPUTATIONAL COMPLEXITY
DOES P≠NP?
PSPACE
NP COMPLETE
NP
BQP
P
EFFICIENT FOR A QUANTUM COMPUTER
EFFICIENT FOR A COMPUTER
INFORMATION THEORY
ENTROPY
ERROR CORRECTION
CODING THEORY
PARITY CHECKING
CRYPTOGRAPHY
PUBLIC KEY
PRIVATE KEY
ALL THE SECRETS
THEORETICAL COMPUTER SCIENCE
COMPUTABILITY THEORY
ALAN TURING
TURING MACHINE
STATE REGISTER
INFINITELY LONG TAPE
HEAD
LAMBDA CALCULUS
GPU
RAM
POWER
MOTHERBOARD
SCHEDULING
PROCESSES
SCHEDULER
MULTIPROCESSING
COMPUTER ARCHITECTURE
CPU
INPUT
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ARITHMETIC/LOGIC UNIT
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FPGA
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LINKED LIST
GRAPH
STACK
HASHING
FORMAL METHODS
POSSIBLE STATES
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C++
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AND
XOR
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GRAPH THEORY
AUTOMATA THEORY
QUANTUM COMPUTATION
AND MORE
PARALLEL PROGRAMMING
MAIN JOB
SMALLER JOBS
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UNIT TESTING
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OBJECT ORIENTED DESIGN
OPERATING SYSTEMS
iOS
macOS
NETWORKING
CONCURRENT/DISTRIBUTED/PARALLEL/SYSTEMS
DATABASES
SQL
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COMPUTER ANALYSIS
BENCHMARKING
OPTIMISATION
FINANCE
LEAGUE OF LEGENDS
AMAZON WAREHOUSE
BOOLEAN SATISFIABILITY
x_1 OR x_2 OR $\bar{x}_3$ (SAT)
SUPER COMPUTING
COMPUTER GRAPHICS
COMPUTATIONAL SCIENCE
COMPUTATIONAL PHYSICS
NUMERICAL ANALYSIS
COMPUTATIONAL CHEMISTRY
HACKING
MACHINE LEARNING
SUPERVISED
UNSUPERVISED
REINFORCEMENT
NEURAL NETWORK
CAT
ARTIFICIAL INTELLIGENCE
A.I.
ROBOTICS
COMPUTER VISION
FIND THE HUMANS
APPLICATIONS
VIRTUAL REALITY
SIMULATION
BIG DATA
NATURAL LANGUAGE PROCESSING
CHATBOTS
-HEY
HELLO THERE-
-ARE U A ROBOT?
YES-
WAIT, I MEAN NO-
-PROVE IT!
CALCULATING...-
I MADE YOU CAKE-
TELEPRESENCE
AUGMENTED REALITY
HUMAN COMPUTER INTERACTION
SCONES
TEA
FLOUR
BUTTER
BIRTHDAY
CAKE
FOOD
BACON
CELEBRATION
PANCAKE
BREAKFAST
KNOWLEDGE REPRESENTATION
IMAGE PROCESSING
INTERNET OF THINGS
YOUTUBE DOMAIN OF SCIENCE MAP OF COMPUTER SCIENCE
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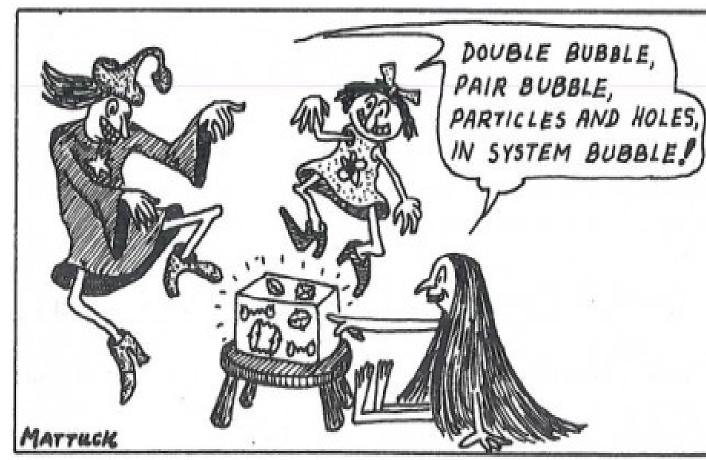
Actors in Material Science

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

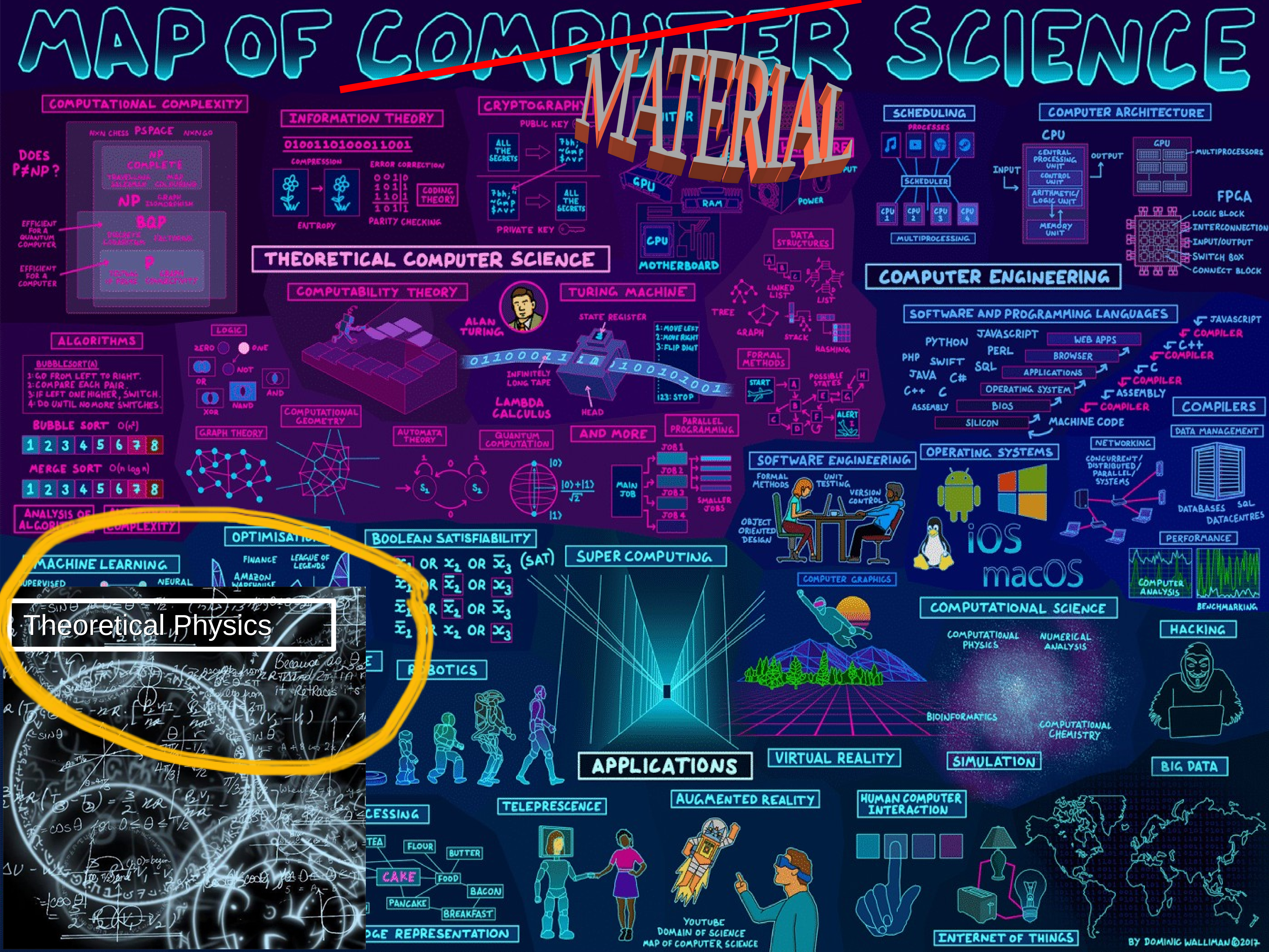
Theoreticians
(Motto: Experimentalists do not understand what they measure)



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

Technical sheet

Model: IBM-BlueGene /Q
Architecture: 10 BGQ Frame with 2 MidPlanes each
Front-end Nodes OS: Red-Hat EL 6.2
Compute Node Kernel: lightweight Linux-like kernel
Processor Type: IBM PowerA2, 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 PFlop/s



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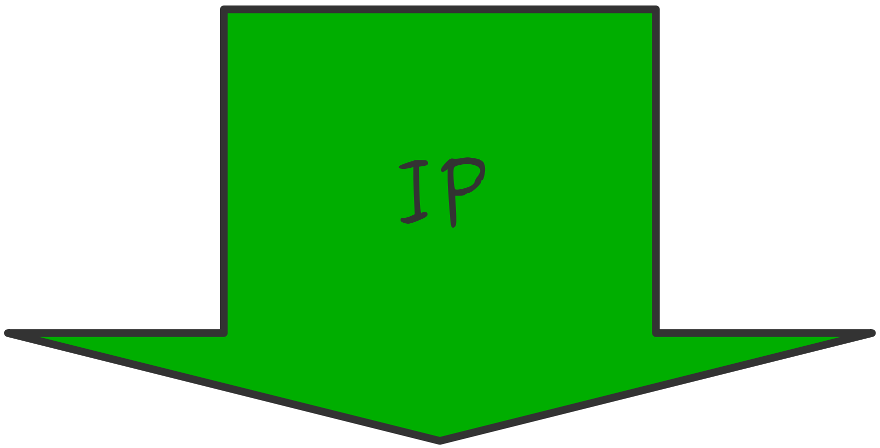
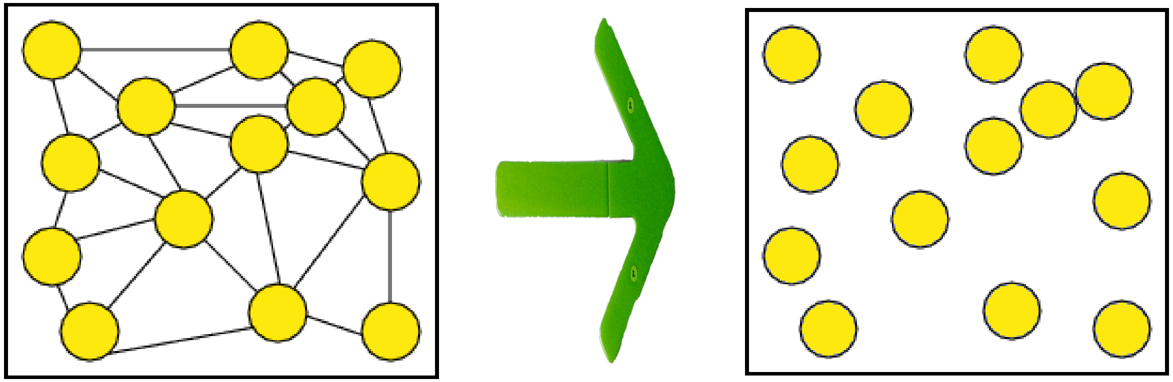
The Many-Body problem (made short)

$$H = \sum_i h(x_i, p_i) + \frac{1}{2} \sum_{i \neq j} |x_i - x_j|^{-1}$$

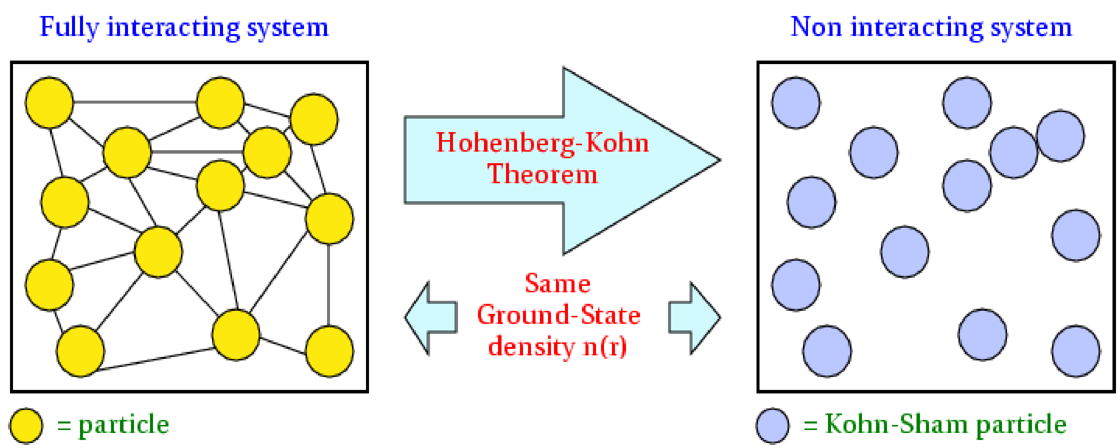




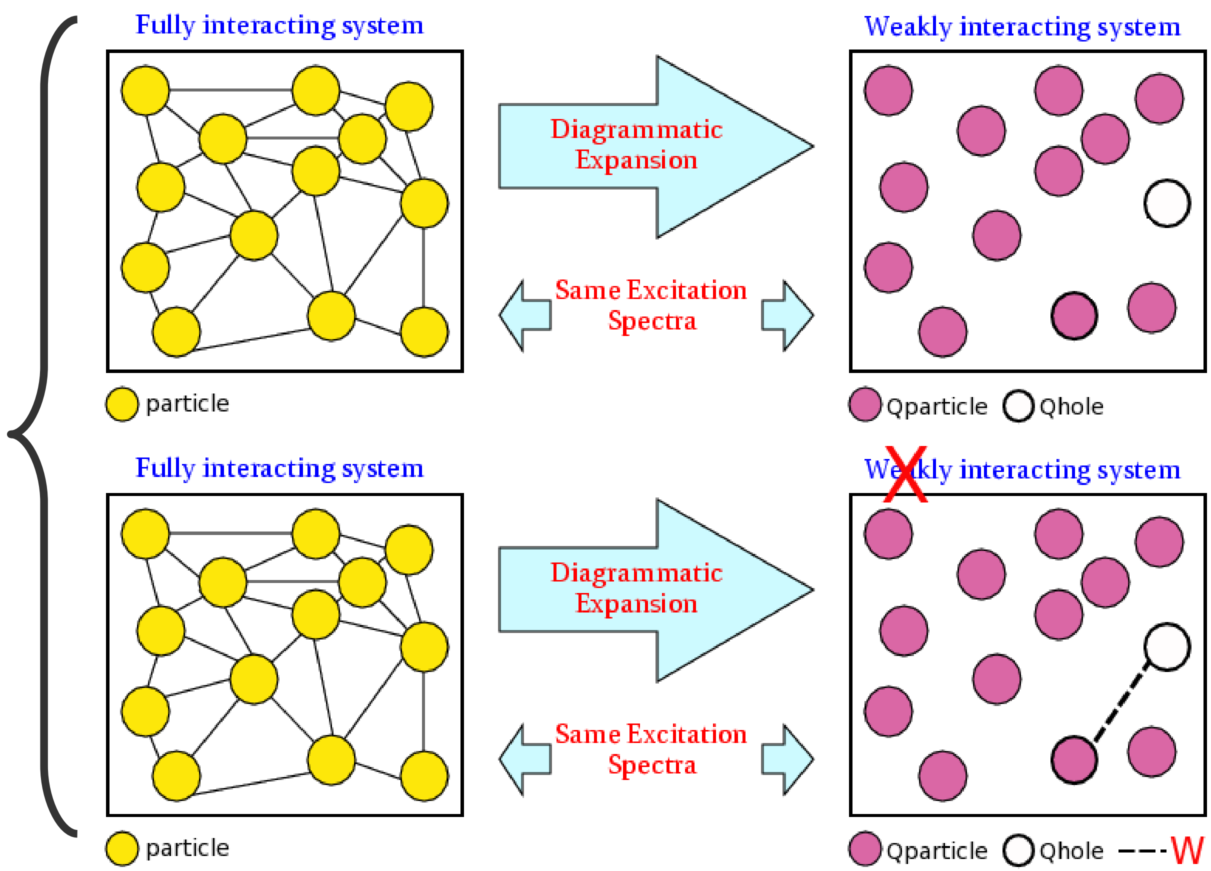
$$H \approx \sum_i h(x_i)$$

The Many-Body problem (made short)

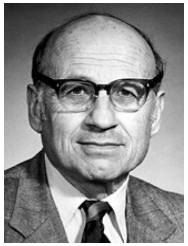
DFT

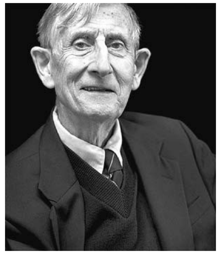


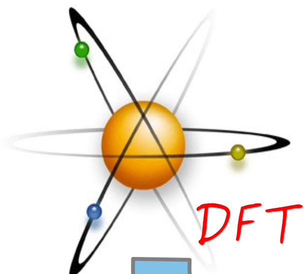
MBPT

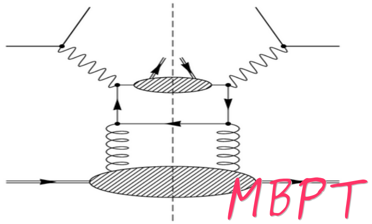


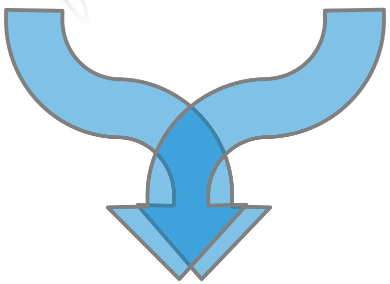
The AiMBPT (Ab-Initio Many-Body Perturbation Theory)

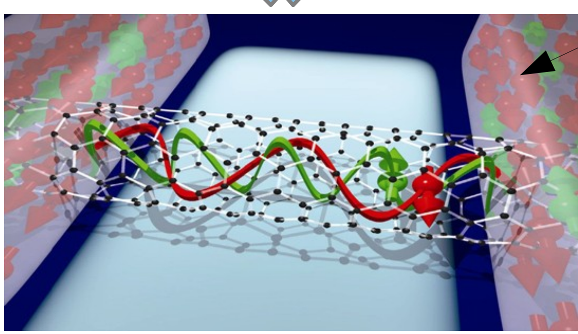












G. Onida, Rev. Mod. Phys. 2002

AiMBPT is...

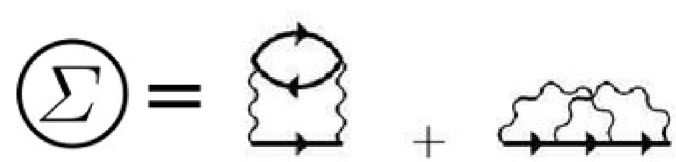
DFT

$$\left[\frac{-\nabla^2}{2}+v_s(r)\right]\psi_{nk}(r)=\epsilon_{nk}\psi_{nk}(r)$$

$$v_s(r)=v_{atoms}(r)+V_{Hxc}(r)$$

+

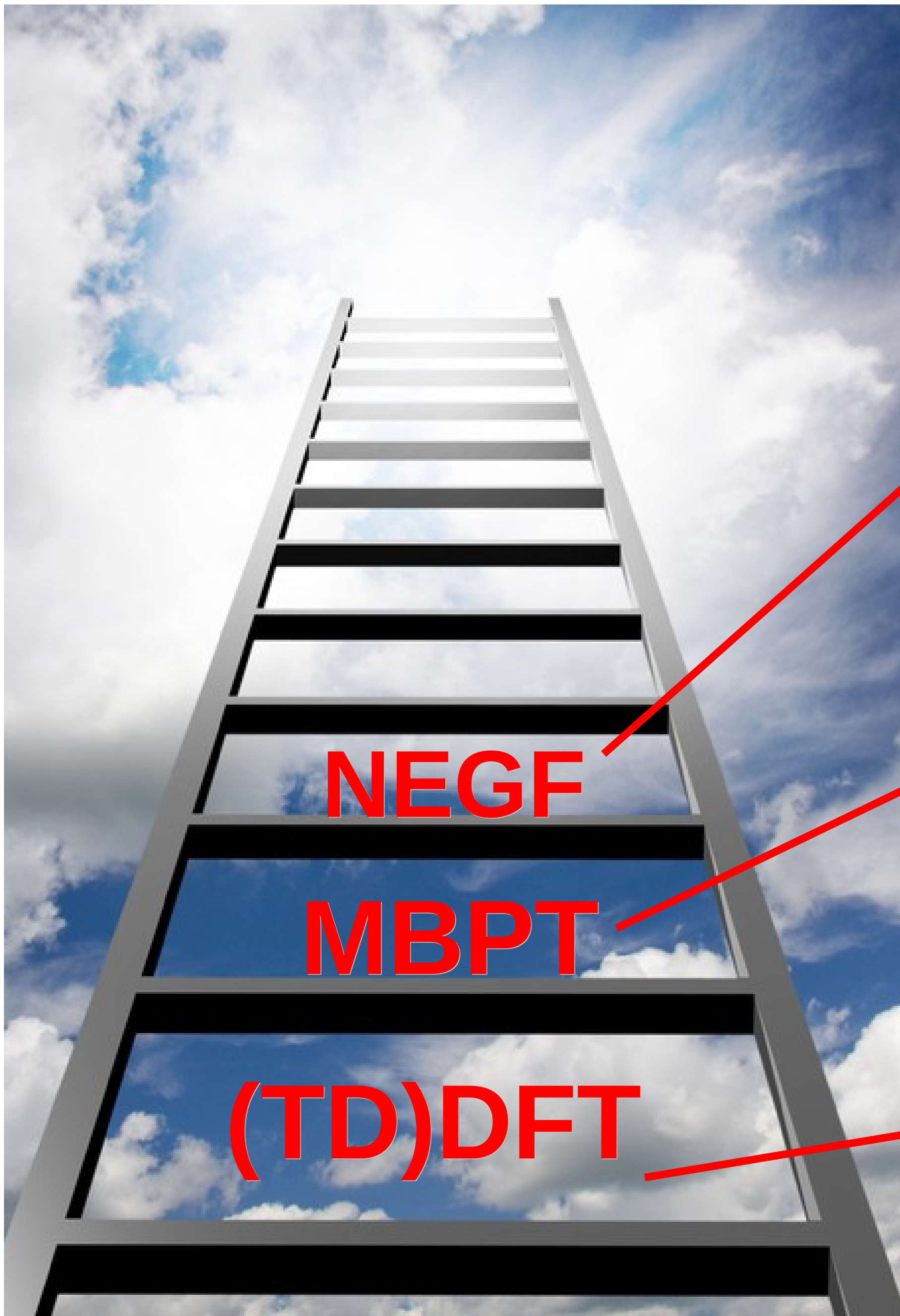
MBPT

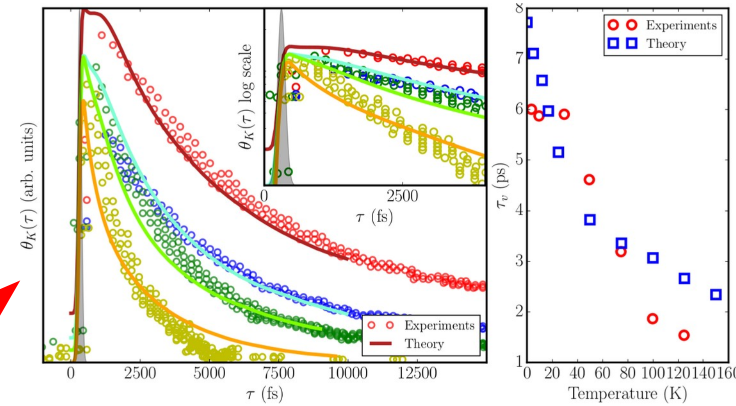


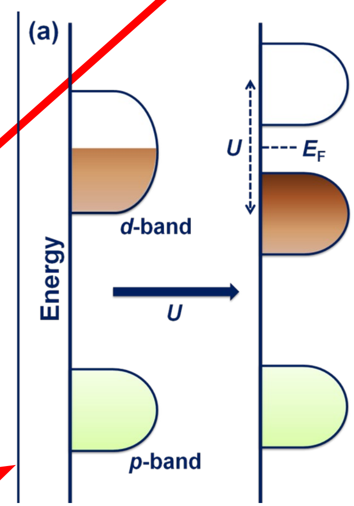
$$G(r_1,r_2;t)\propto\langle T\{\psi(r_1,t)\psi^{+}(r_2)\}\rangle$$

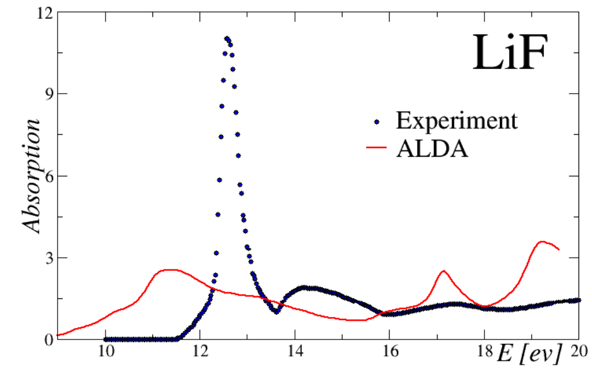
✓ Predictive ✓ Parameter free ✓ Universal ✓ Accurate

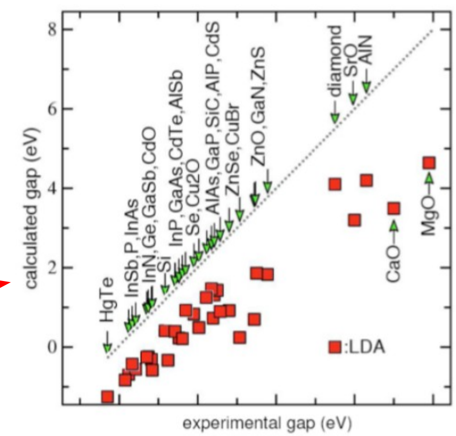
The Ab-Initio "Way"







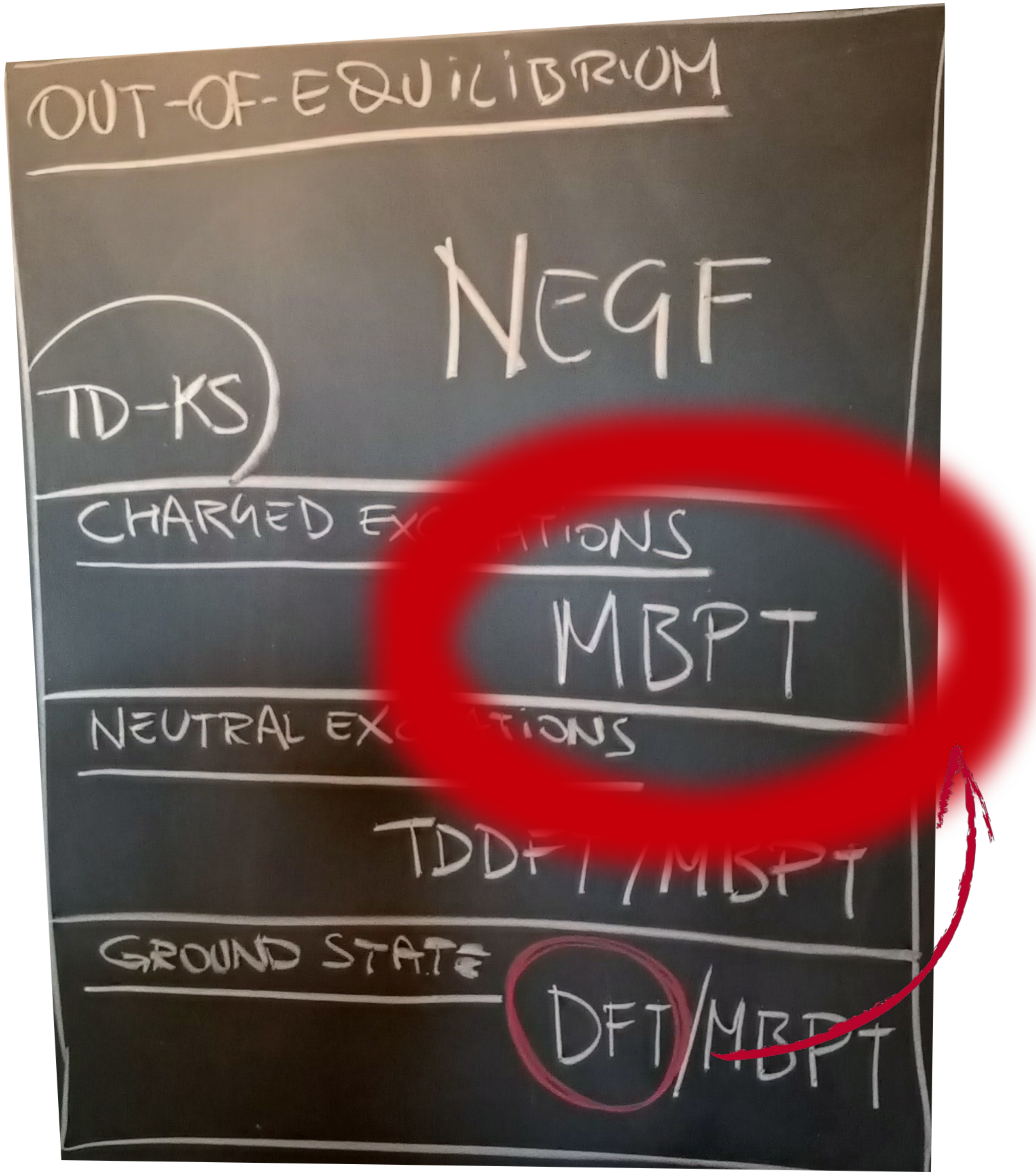




Si:
0.47 eV (LDA) vs 1.1 eV (expt)

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

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

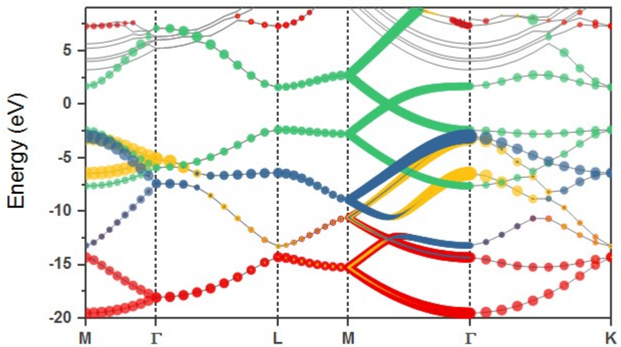


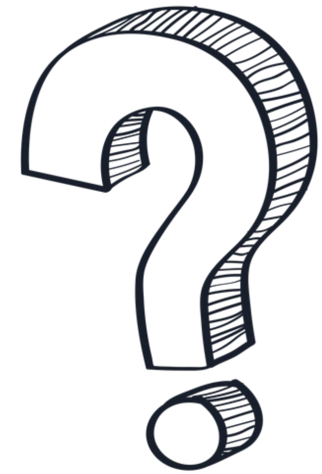
Many-Body Perturbation Theory for dummies

The Many-Body problem

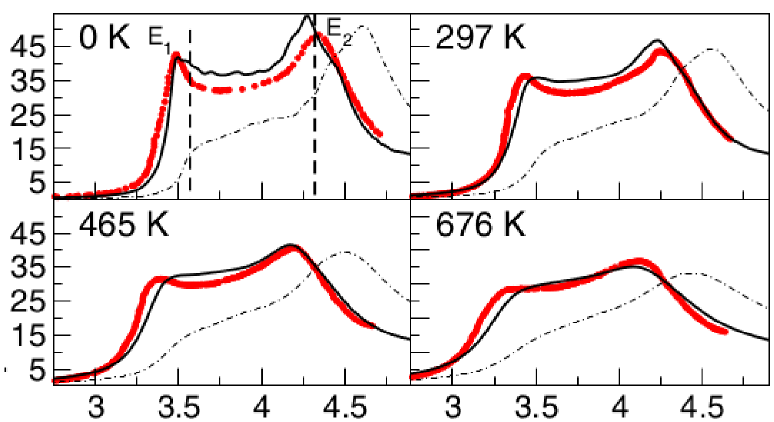
$$H = \sum_i h(x_i, p_i) + \frac{1}{2} \sum_{i \neq j} \left| x_i - x_j \right|^{-1}$$

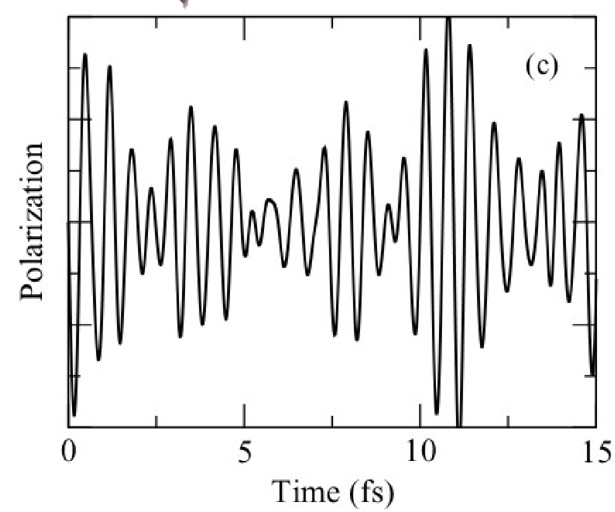
The Many-Body Problem: a micro-macro connection





$$H = \sum_i h(x_i, p_i) + \frac{1}{2}\sum_{i \neq j} |x_i - x_j|^{-1}$$

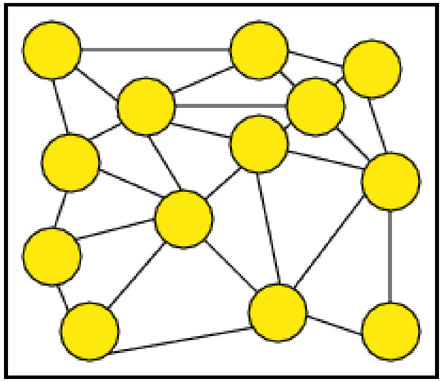




The Many-Body problem: 1 particle approx

$$H = \sum_i h(x_i) + \frac{1}{2}\sum_{i \neq j} |x_i - x_j|^{-1}$$

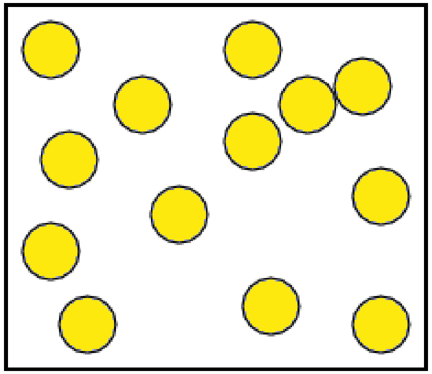
$$H = \sum_i h(x_i)$$



$$\hat{h}|n\rangle = \epsilon_n |n\rangle$$

$$|N\rangle \approx D_N[\{|n\rangle\}]$$

$$|N=0\rangle \approx \prod_n^{(filled)} |n\rangle$$

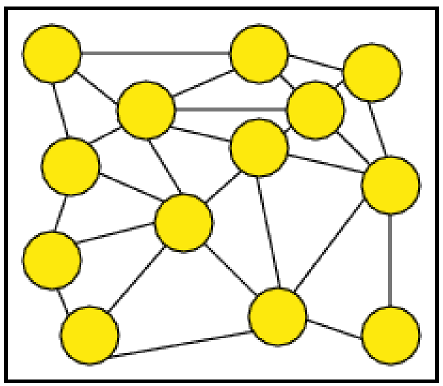


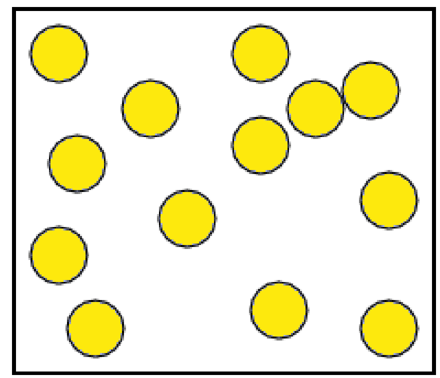
$$\langle N|\hat{A}|N\rangle \approx F_N[\{A_n\}]$$

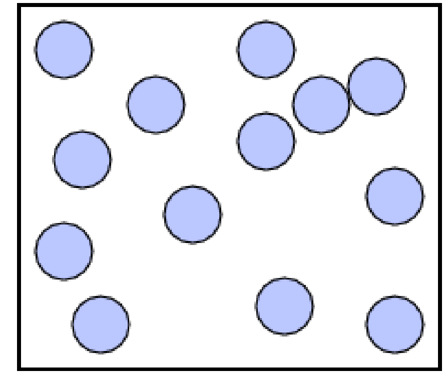
$$\langle N=0|\hat{H}|N=0\rangle \approx \sum_n \epsilon_n$$

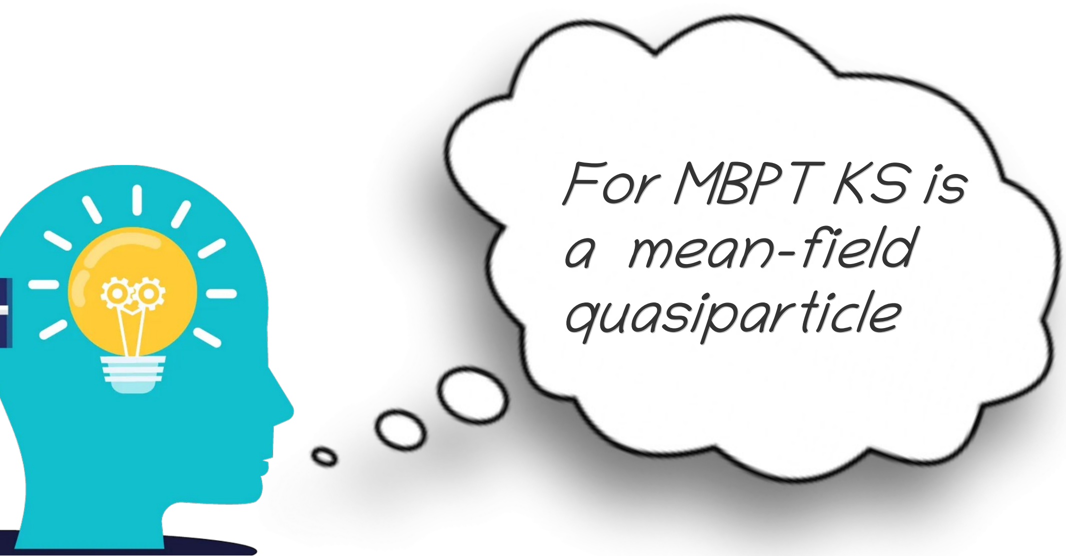
Quasiparticles...

$$H = \overbrace{\sum_i h(x_i)}^{\hat{H}_0} + \frac{1}{2}\sum_{i \neq j} \left| x_i - x_j \right|^{-1} = h + H'$$









The goal of the Many Body methods is to rewrite the fully interacting problem as an as much independent as possible counter-part

The MBPT approach to the TD density

$$n(\mathbf{r},t) = \left\langle \Psi(t) \left| \hat{\psi}^\dagger(\mathbf{r})\hat{\psi}(\mathbf{r}) \right| \Psi(t) \right\rangle$$

Ground State

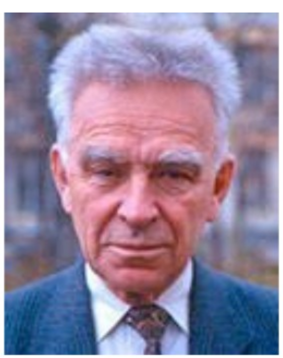
Density Functional Theory

$$\hat{\psi}(\mathbf{r}) = \sum_{\mathbf{k}} \phi_{\mathbf{k}}(\mathbf{r}) \hat{d}_{\mathbf{k}}$$

$$|\,\Psi(t)\rangle = \hat{U}(t,t_0)\ |\,\Psi(t_0)\rangle \longrightarrow \hat{U}(t,-\infty)\ |\,\Phi\rangle$$

Adiabatic Hypothesis

$$\hat{U}(t) \equiv \hat{U}(t,-\infty)$$



$$n(\mathbf{r},t) = \sum_{\mathbf{k}\mathbf{k}'} \phi^*_{\mathbf{k}}(\mathbf{r})\phi_{\mathbf{k}'}(\mathbf{r}) \left\langle \Psi(t) \left| \hat{d}^\dagger_{\mathbf{k}} \hat{U}(t) \hat{U}^\dagger(t) \hat{d}_{\mathbf{k}'} \right| \Psi(t) \right\rangle$$

The evolution operator (scattering potential)

$$\hat{H}(t) = \hat{H}_0 + \hat{V}(t)$$

⇓

$$i\frac{d}{dt}\hat{U}_0(t) = \hat{H}_0\hat{U}_0(t)$$

⇓

$$\hat{U}(t) = \hat{U}_0(t)\hat{F}(t)$$

⇓

$$\hat{F}(t) = 1 - i\int_{-\infty}^{t} dt_1 \hat{V}_I(t_1) + (-i)^2 \int_{-\infty}^{t} dt_1 \int_{-\infty}^{t_1} dt_2 \hat{V}_I(t_1)\hat{V}_I(t_2) + \ldots$$

Constrained time integrals

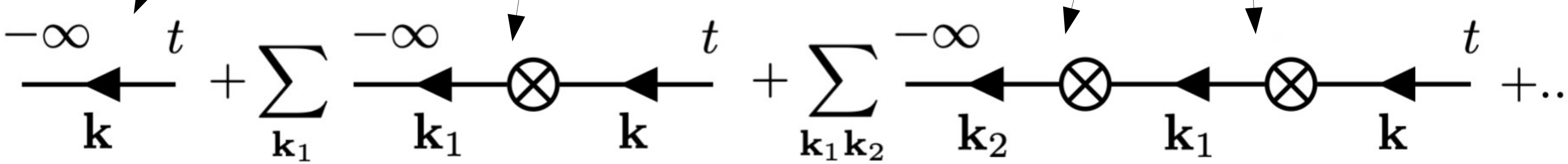
$t > t_1 > t_2 > \cdots$

Half the dynamics...

$$\left\langle \Psi(t) \left| \hat{d}^\dagger_{\mathbf{k}} \hat{U}(t) \hat{U}^\dagger(t) \hat{d}_{\mathbf{k}'} \right| \Psi(t) \right\rangle = \delta_{\mathbf{k}\mathbf{k}'} - \left\langle \Psi(t) \left| \hat{d}^\dagger_{\mathbf{k}} \hat{U}(t) \hat{U}^\dagger(t) \hat{d}^\dagger_{\mathbf{k}'} \right| \Psi(t) \right\rangle$$

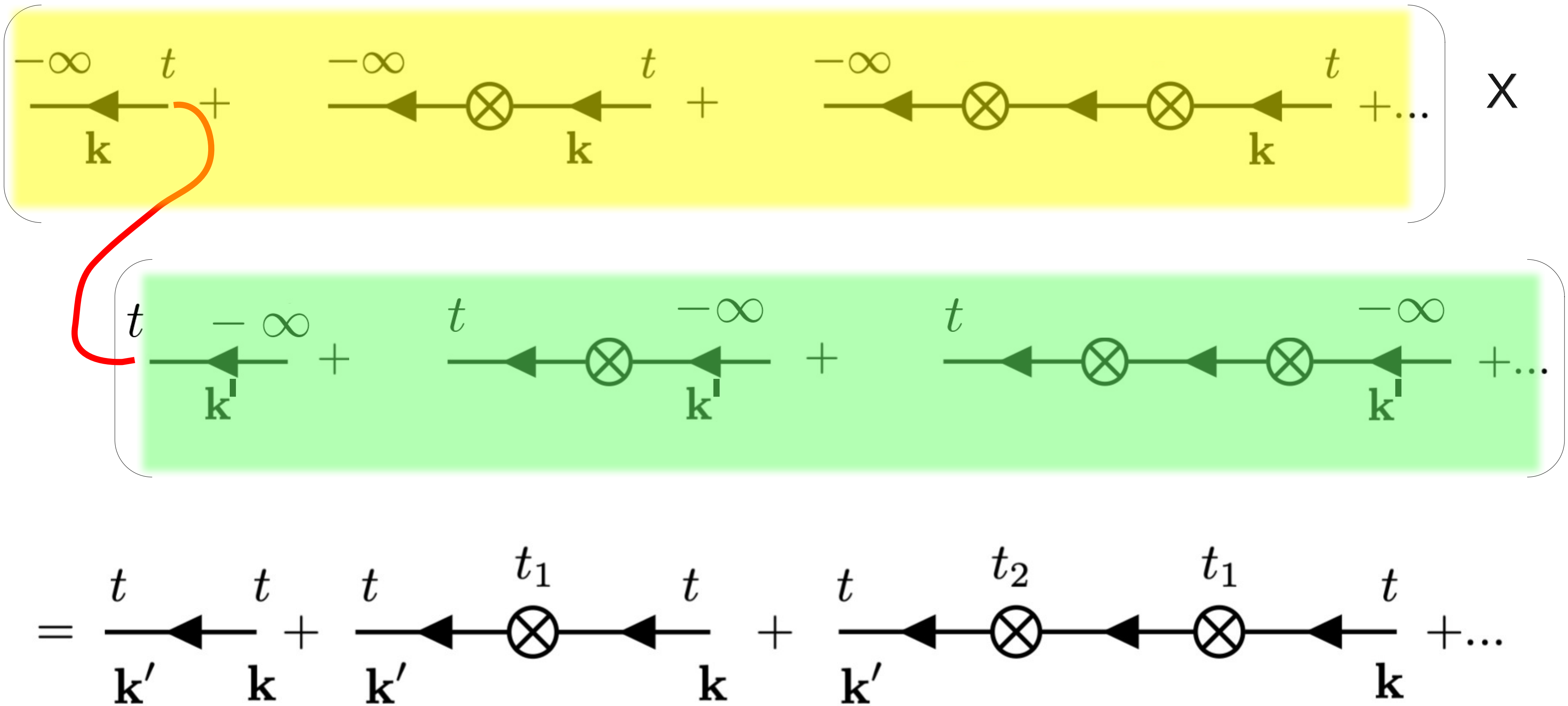
$$\hat{U}^\dagger(t) \hat{d}^\dagger_{\mathbf{k}} \left| \Psi(t) \right\rangle = F^\dagger(t) \hat{U}^\dagger_0(t) \hat{d}^\dagger_{\mathbf{k}} \left| \Psi(t) \right\rangle$$

$$\hat{F}(t) = 1 + i \int_{-\infty}^{t} dt_1 \hat{V}_I(t_1) + i^2 \int_{-\infty}^{t} dt_1 \int_{-\infty}^{t_1} dt_2 \hat{V}_I(t_2) \hat{V}_I(t_1) + \dots$$



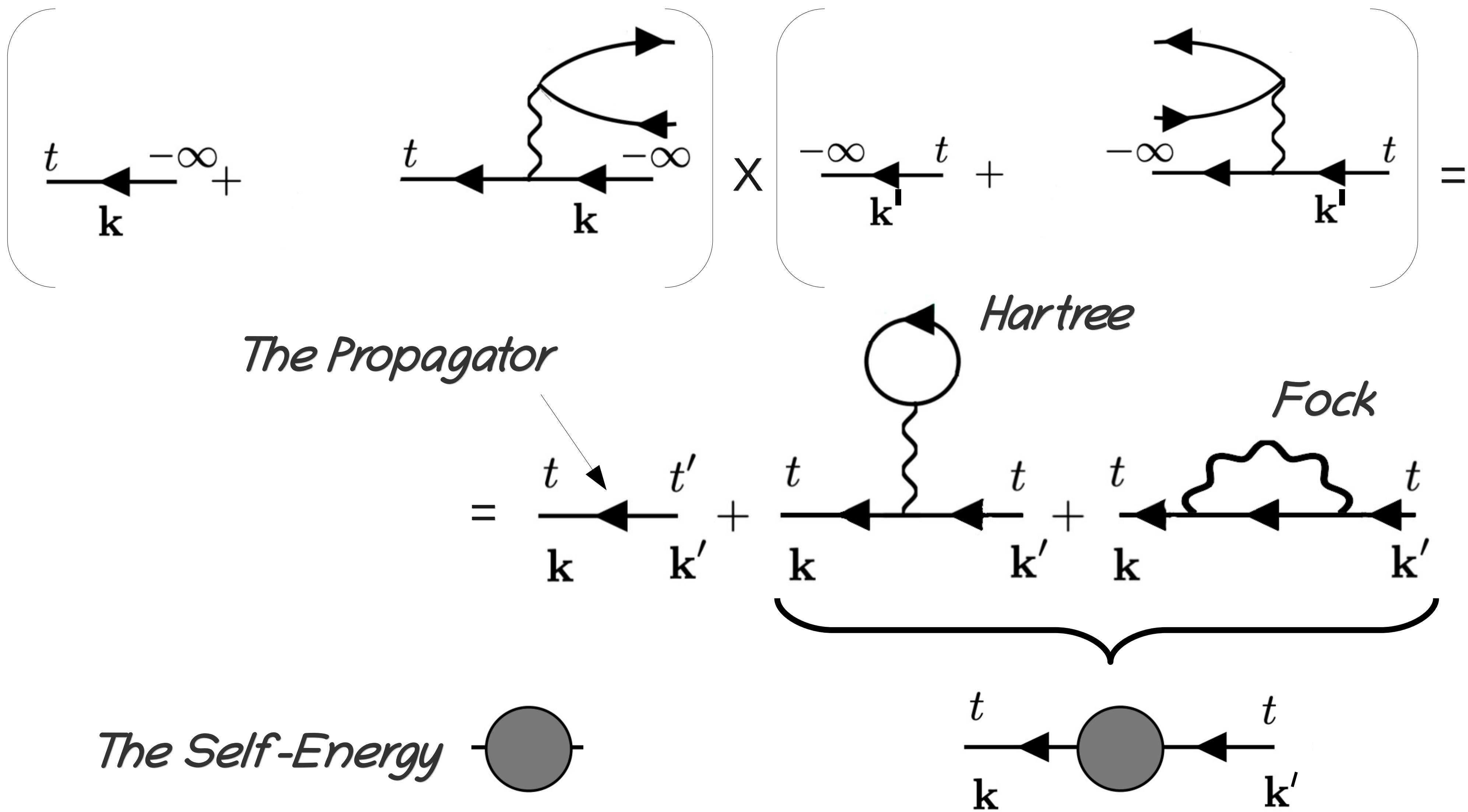
Green's Functions

$$\left\langle \Psi(t) \left| \hat{d}^{\dagger}_{\mathbf{k}} \hat{U}(t) \hat{U}^{\dagger}(t) \hat{d}^{\dagger}_{\mathbf{k}'} \right| \Psi(t) \right\rangle =$$

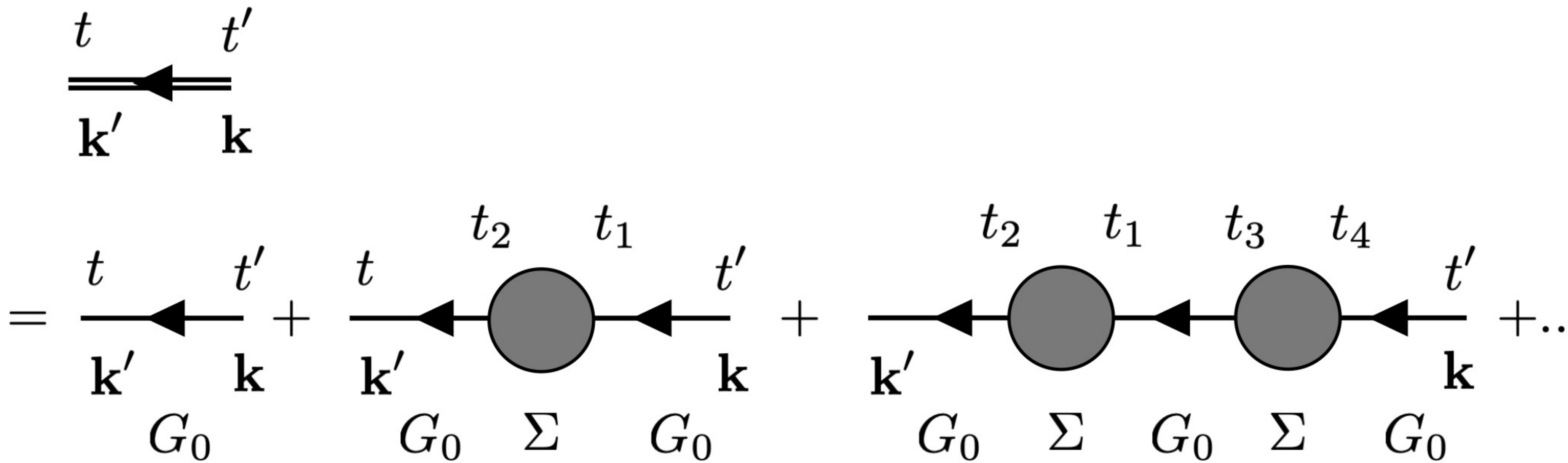


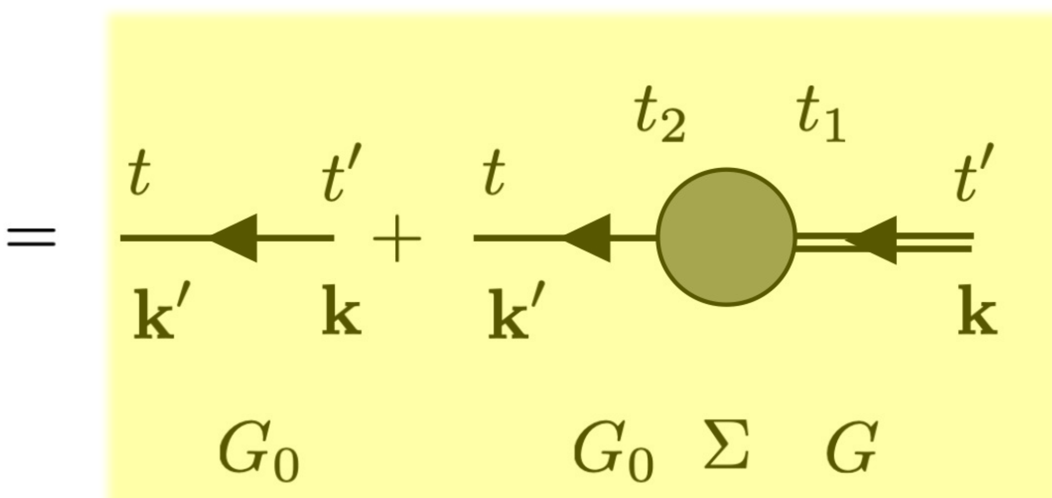
Feynman diagrams in the fully interacting case

$$\left\langle \Psi(t) \left| \hat{d}^{\dagger}_{\mathbf{k}} \hat{U}(t) \hat{U}^{\dagger}(t) \hat{d}^{\dagger}_{\mathbf{k}'} \right| \Psi(t) \right\rangle =$$



The Dyson equation





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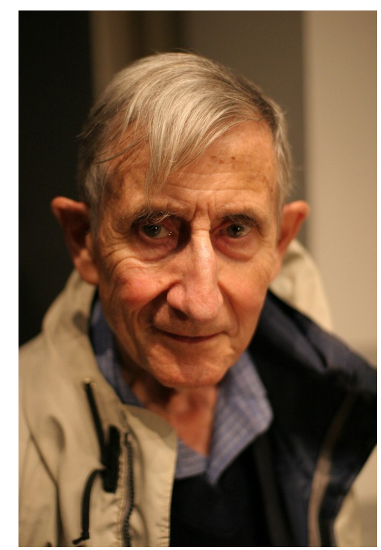
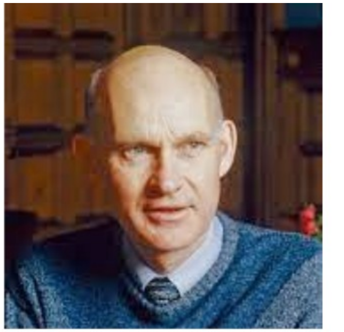
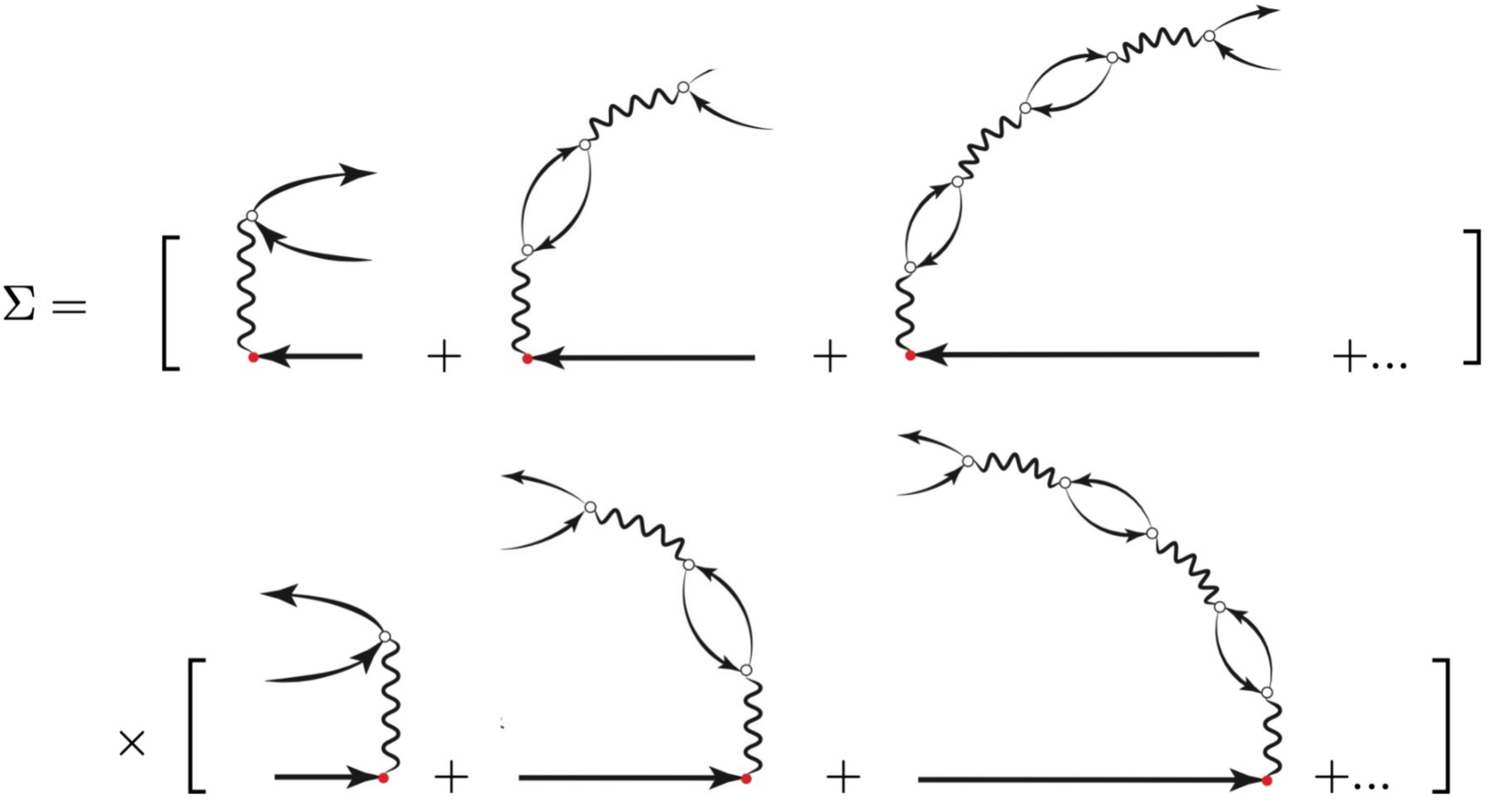


The GW approximation

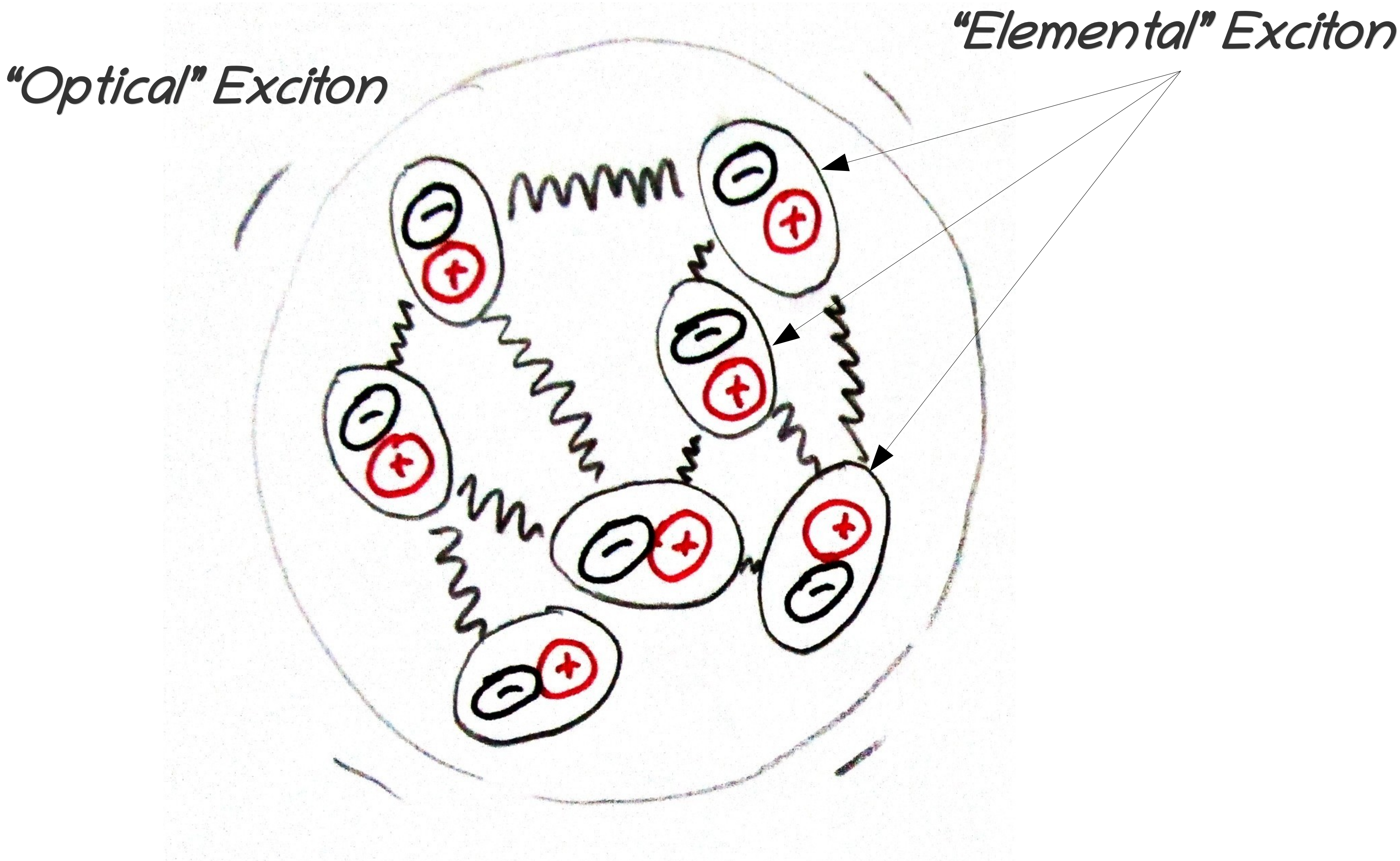




A quick view on an advanced MBPT application

"Optical" vs "Elemental" Excitons

F. Paleari and AM, Phys. Rev. B 106, 125403 (2022)



Exciton-Phonon scattering reveals the excitonic "internal structure"

Yambo: from MBPT to GPU's

The Yambo project

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

4

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).

20

YAMBO is an open-source code released within the GPL licence implementing first-principles methods based on Green's function theory to describe excited-state properties of realistic materials. These methods include the GW approximation, the Bethe-Salpeter equation (BSE), electron-phonon interaction and non-equilibrium Green's function theory (NEGF).

www.yambo-code.eu

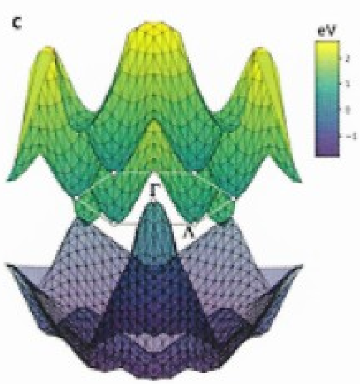
The Yambo project

Level of theory

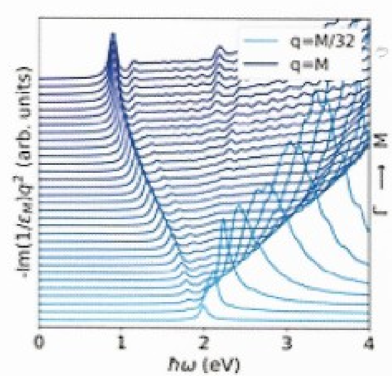
- Many-body perturbation theory (MBPT), incl. GW, BSE
- Electron-phonon coupling (ELPH)
- Real-time non-equilibrium Green's function (NEGF)
- Time Dependent DFT (TDDFT)

Features

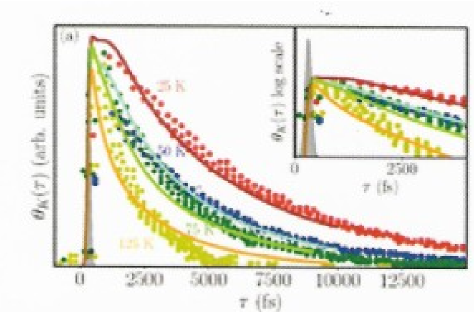
- Electronic properties: quasi-particle energies, line-widths, and renormalization factors
- Linear optical properties, capturing the physics of excitons, plasmons, and magnons
- Temperature dependent electronic and optical properties via electron-phonon coupling
- Non-equilibrium and Non-linear optical properties via NEGF real-time simulations
- Calculation of 2D and 1D systems
- Advanced post-processing tools to analyse the simulation flow of data



Quasiparticle band structure of bulk MoS2 at ultra-high pressure [Ataei et al. Pnas (2021)]

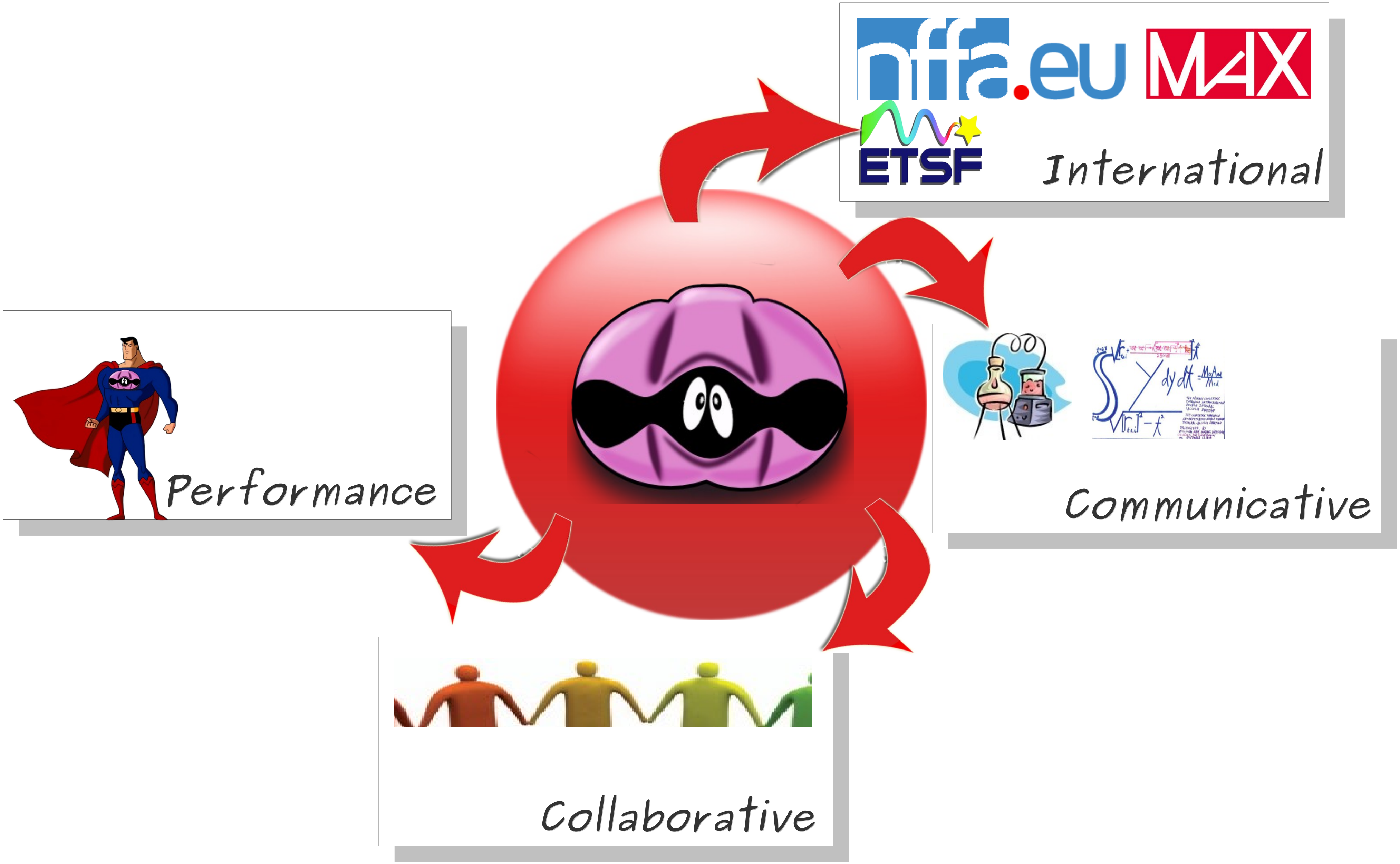


Excitonic EELS spectra at finite momenta of monolayer C3N [Bonacci et al. Phys rev. Mat (2022)]

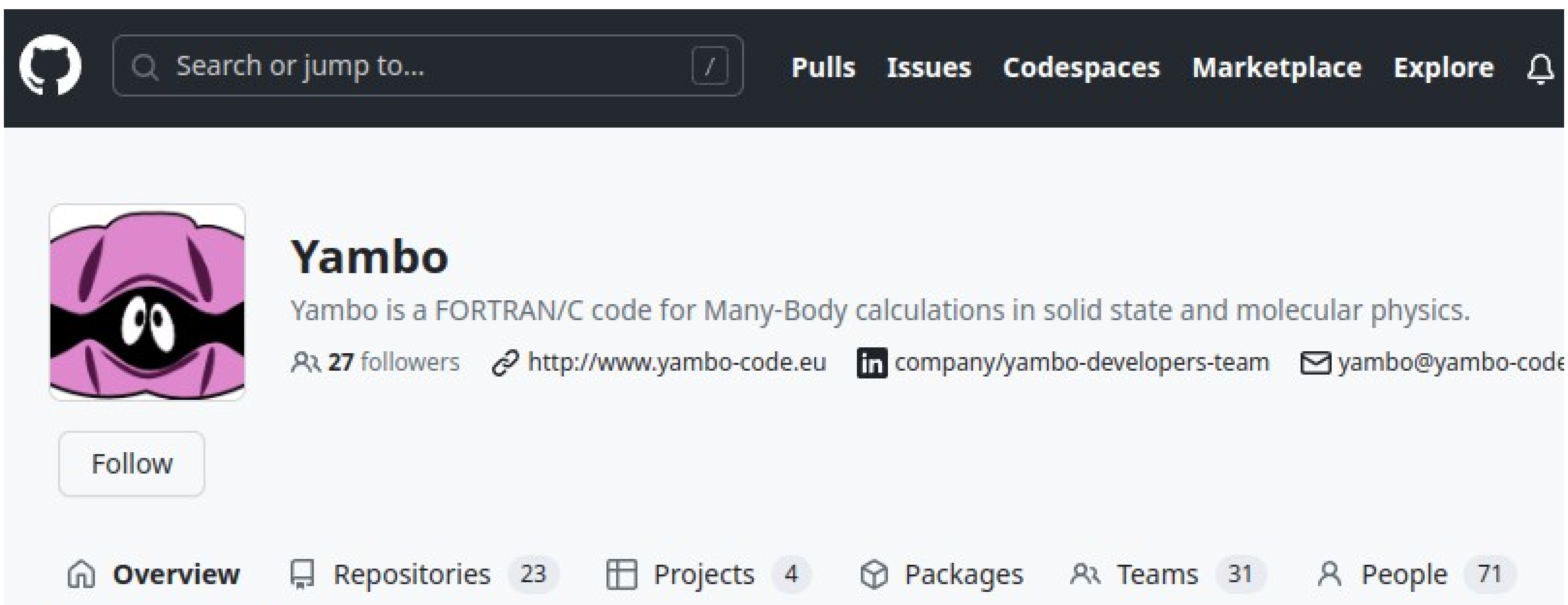


Intervalley relaxation dynamics of monolayer WSe2 via ELPH scattering [Molina-Sánchez et al. Nano Lett. (2017)]

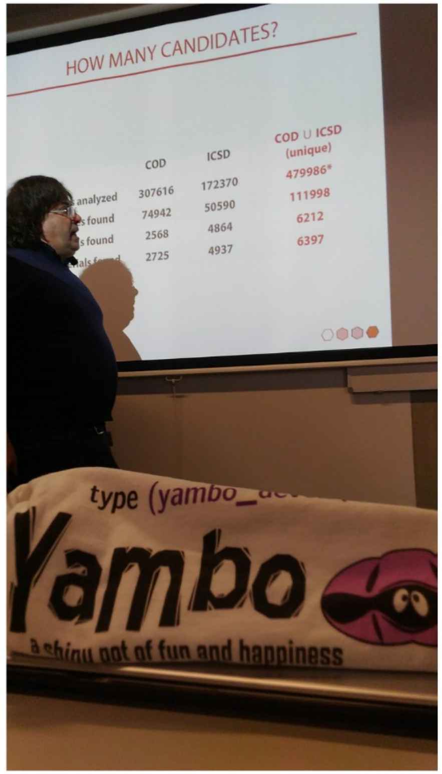
The Yambo project



Be collaborative



Dissemination



2008	Spain
2010	Spain, Italy
2011	Brazil
2012	Spain, Switzerland
2013	Italy, UK, Switzerland
2014	Italy, Japan
2015	Switzerland, South Africa
2016	Italy, Ghana
2017	Italy, Switzerland
2018	Italy, Ethiopia
2019	Cameroon, Crete
2020	(ZOOM)
2021	-
2022	Congo, ICTP
2023	Kenya, Rome. Rwanda

Dissemination

Main page | Discussion | Read | View source | View history | Search The Yambo Projec

- Edu Home
- WWW Home
- Tutorials
- download
- Install
- Virtual Machines (Cloud, docker, VBox)
- Developers Corner

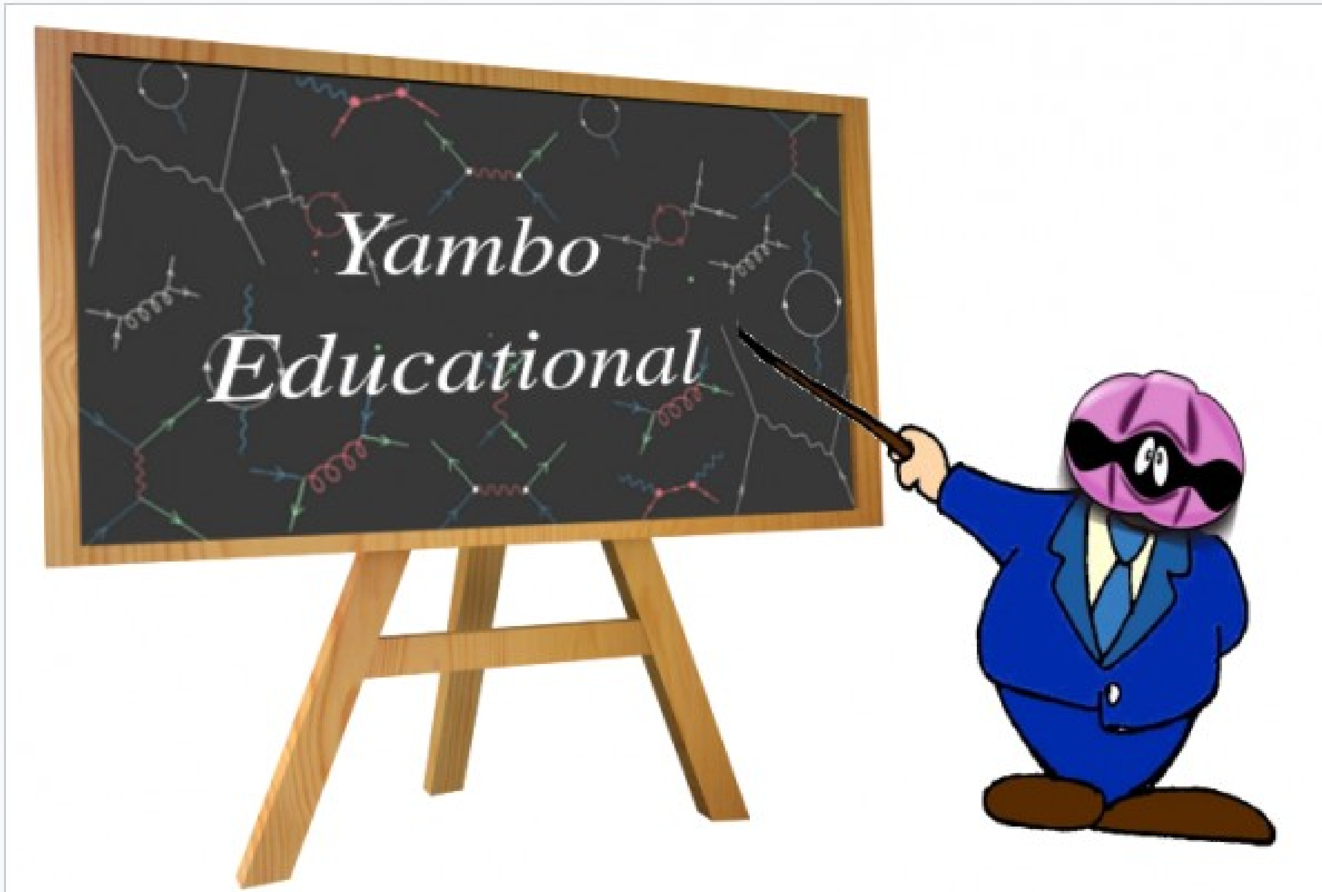
Read!

- Theory
- Lectures
- Cheatsheets
- Selected Readings
- Thesis

Learn! (Modular Tutorials)

- Overview
- Files Download
- First steps
- GW basics
- GW in parallel
- GW convergence

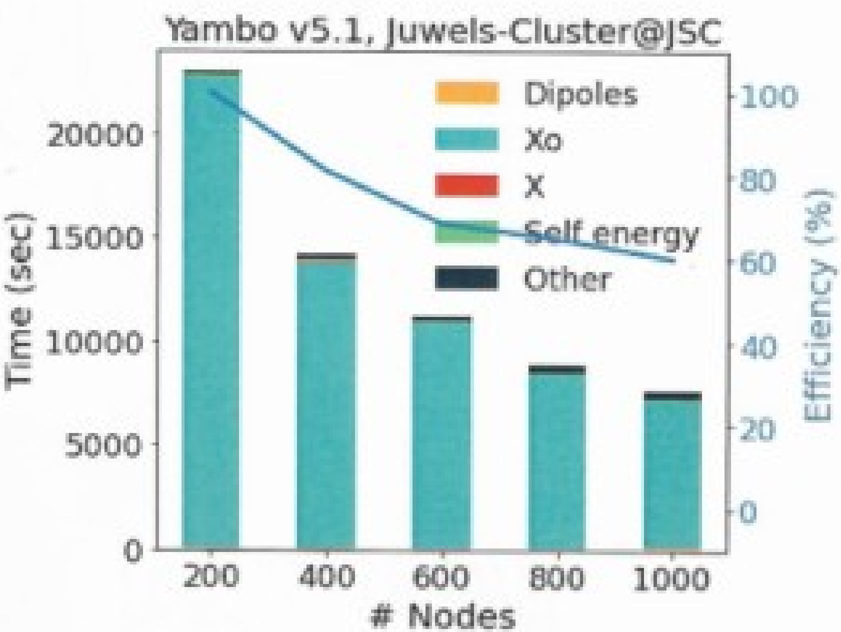
Main Page



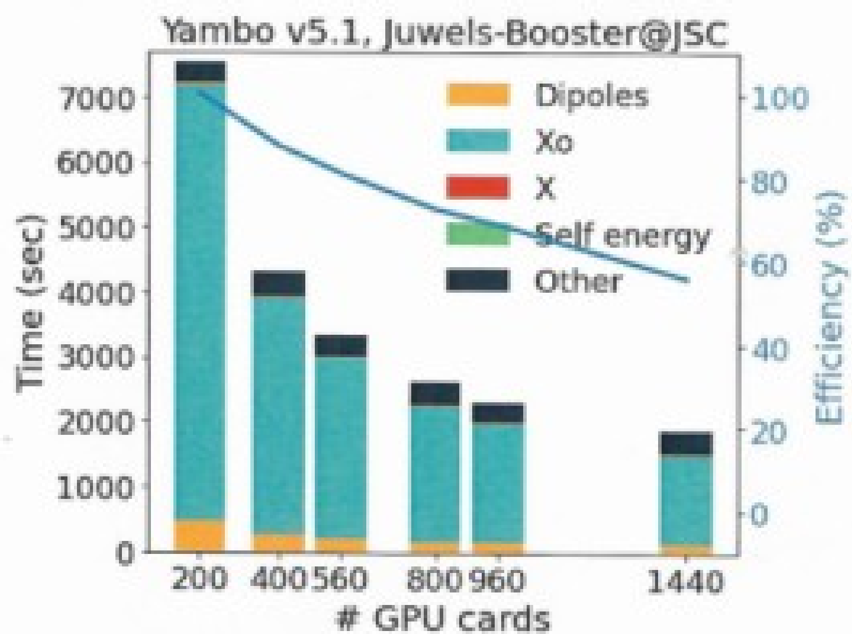
Welcome to the Yambo educational page. In this page you will find several informations about how to run Yambo and, more generally, about the methods implemented in the code.

Parallelization and Performance

Yambo has a user-friendly command-line interface, flexible I/O procedures, and, concerning high performance computing (HPC), it is parallelised by using a hybrid MPI plus OpenMP approach, well integrated with support of GPGPU-based heterogeneous architectures. This makes it possible to distribute the workload to a large number of parallel levels. In practice, depending on the kind of calculation, all the variables to be used (k/q grids, bands, quasi-particles, G-vectors, etc) are distributed along the different levels of parallelisation.

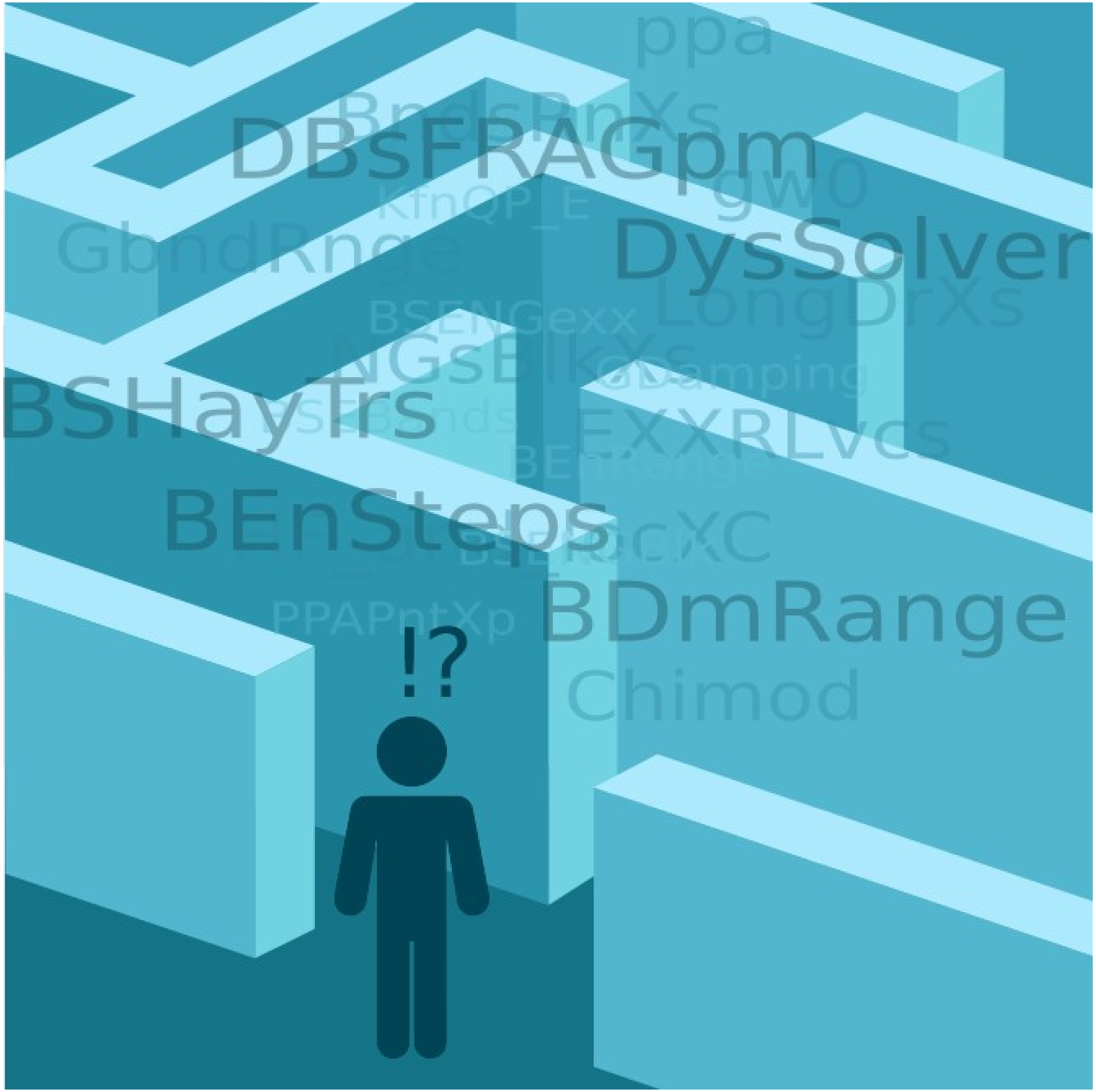


Yambo has proved to be efficient in large-scale simulations (tens of thousands of MPI tasks combined with OpenMP parallelism) for most of its calculation environments. The GPU porting supports CUDA-Fortran as well as other programming models (OpenACC and OpenMP5 under development). Yambo has been demonstrated to run efficiently on a number of HPC architectures, including homogeneous clusters (e.g., based on Intel, AMD, IBM Power and ARM chips), as well as heterogeneous GPU-accelerated machines (currently based on NVIDIA cards).



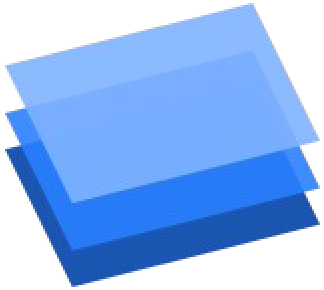
The scientific Method

The path from mistery to mastery



How to go from mistery to mastery

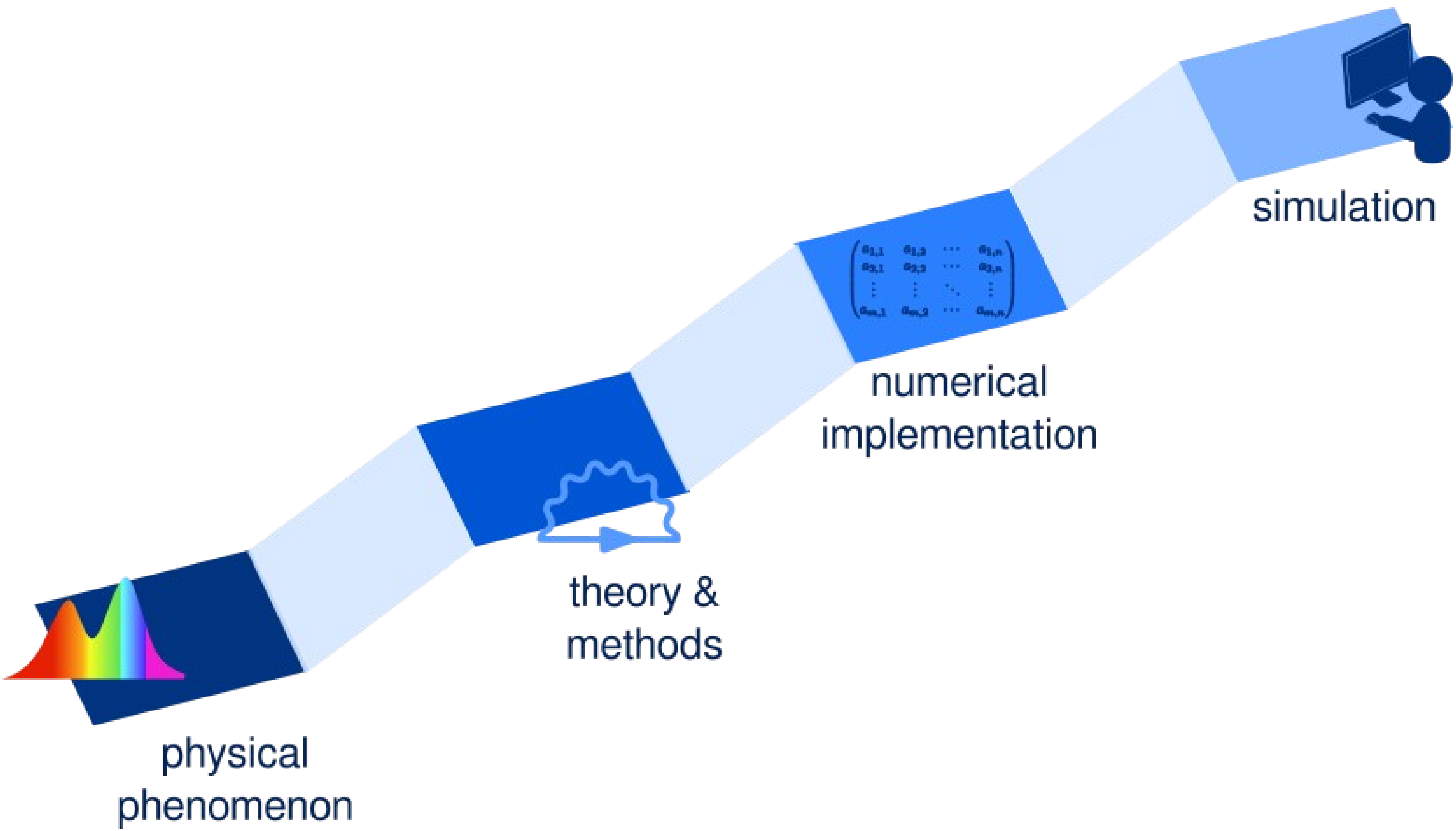
Understand levels of complexity



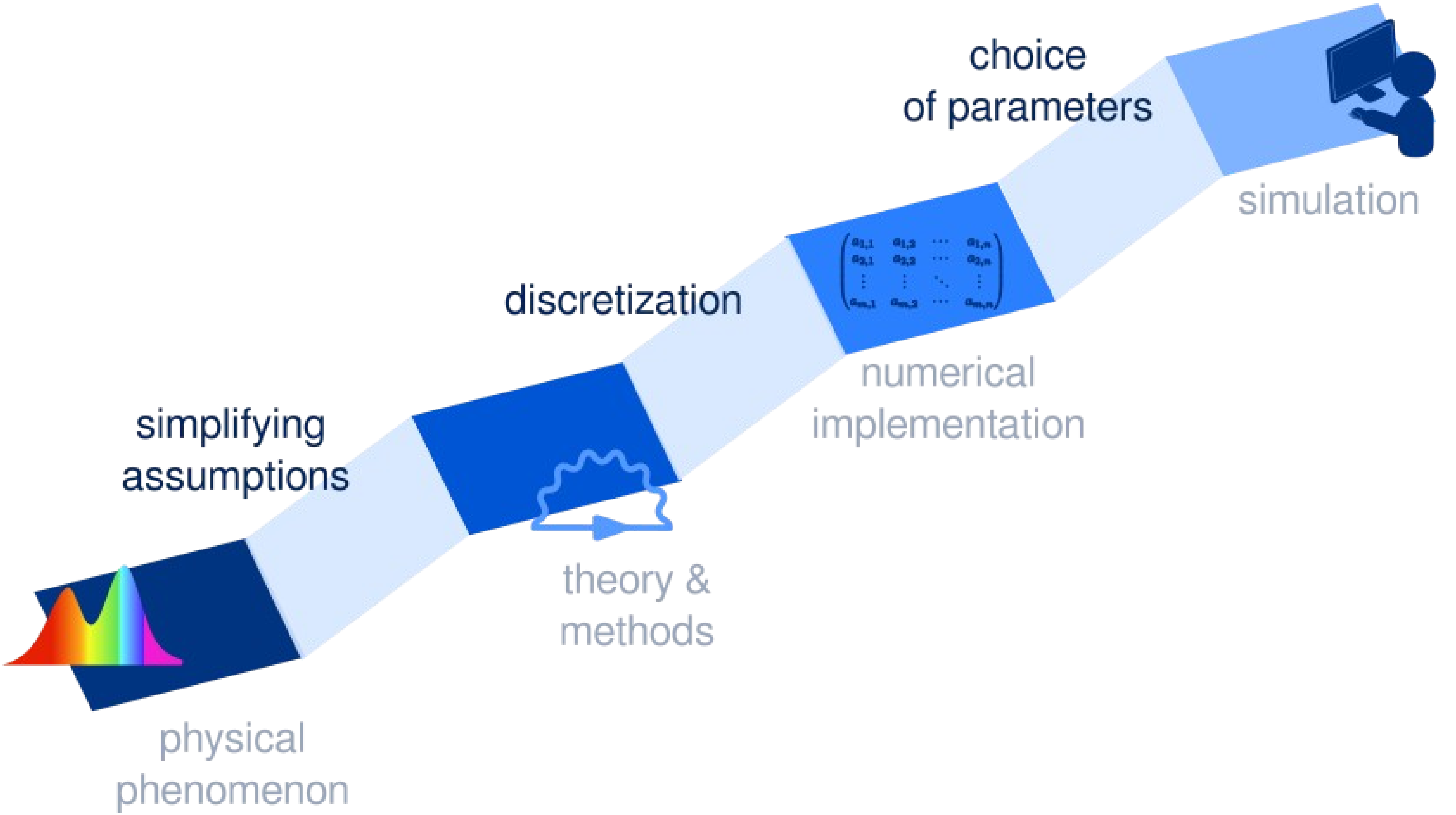
Read & study theory

Learn through hands-on tutorials

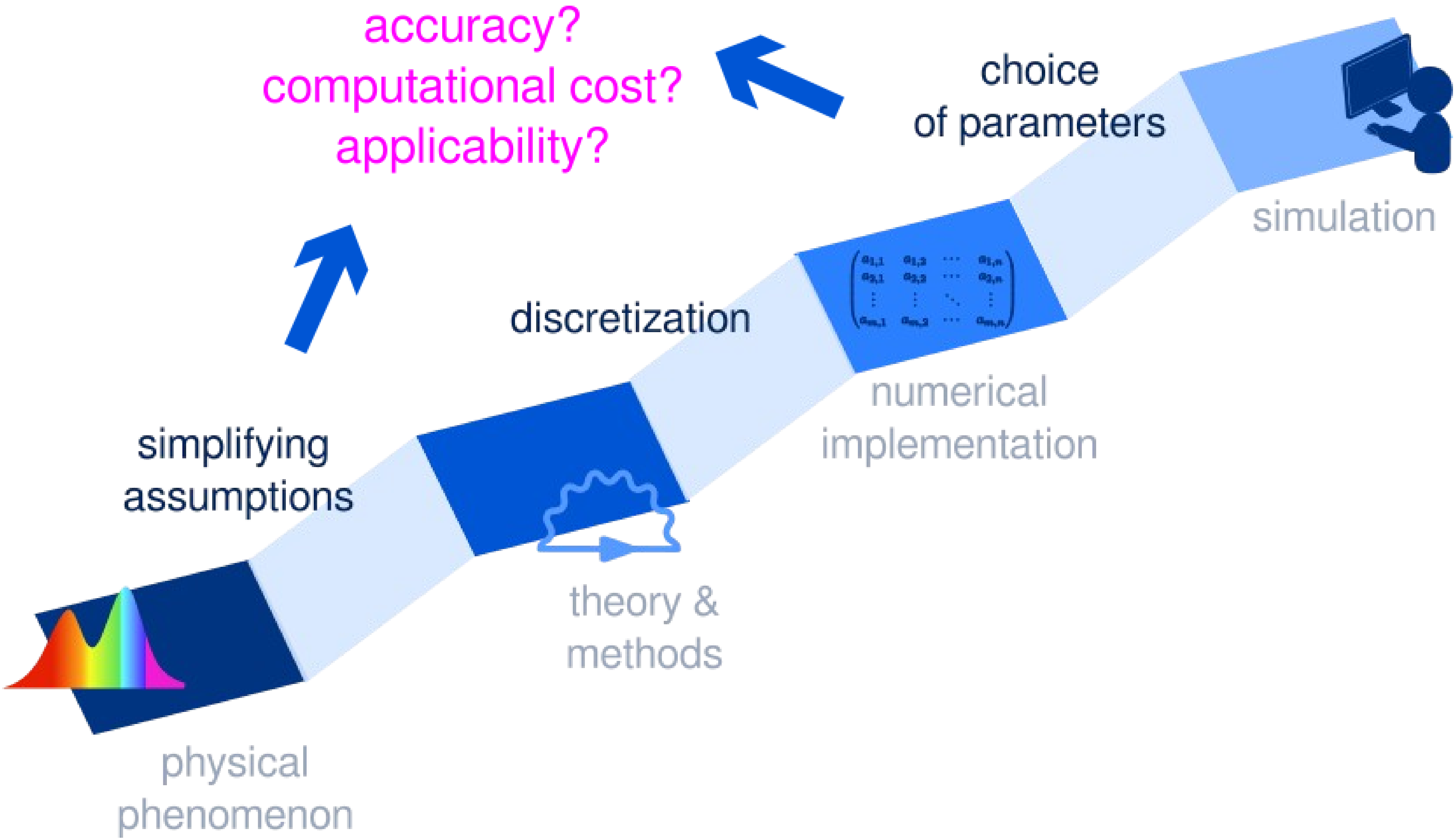
What is behind 'running a simulation'?



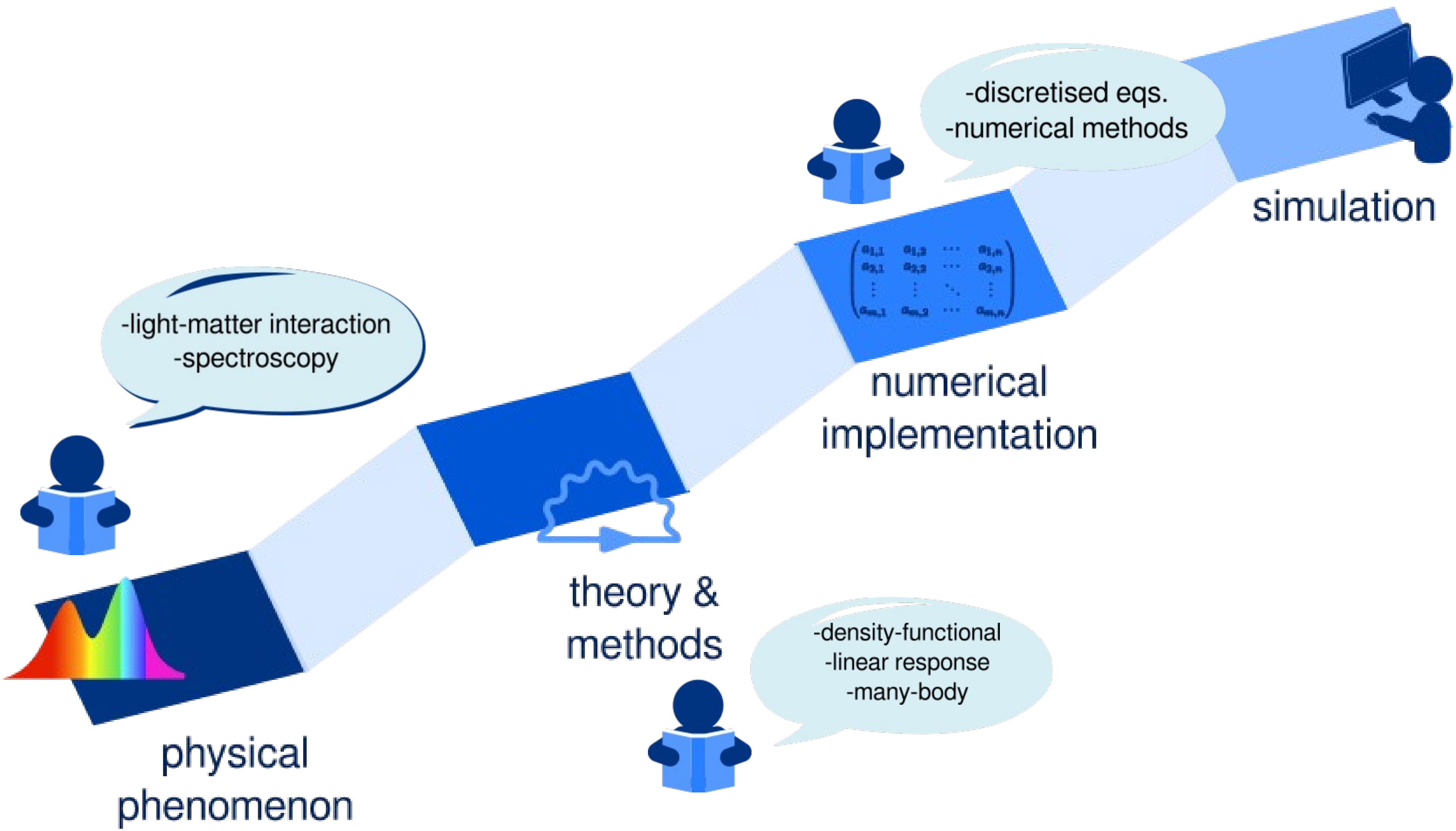
What is behind 'running a simulation'?



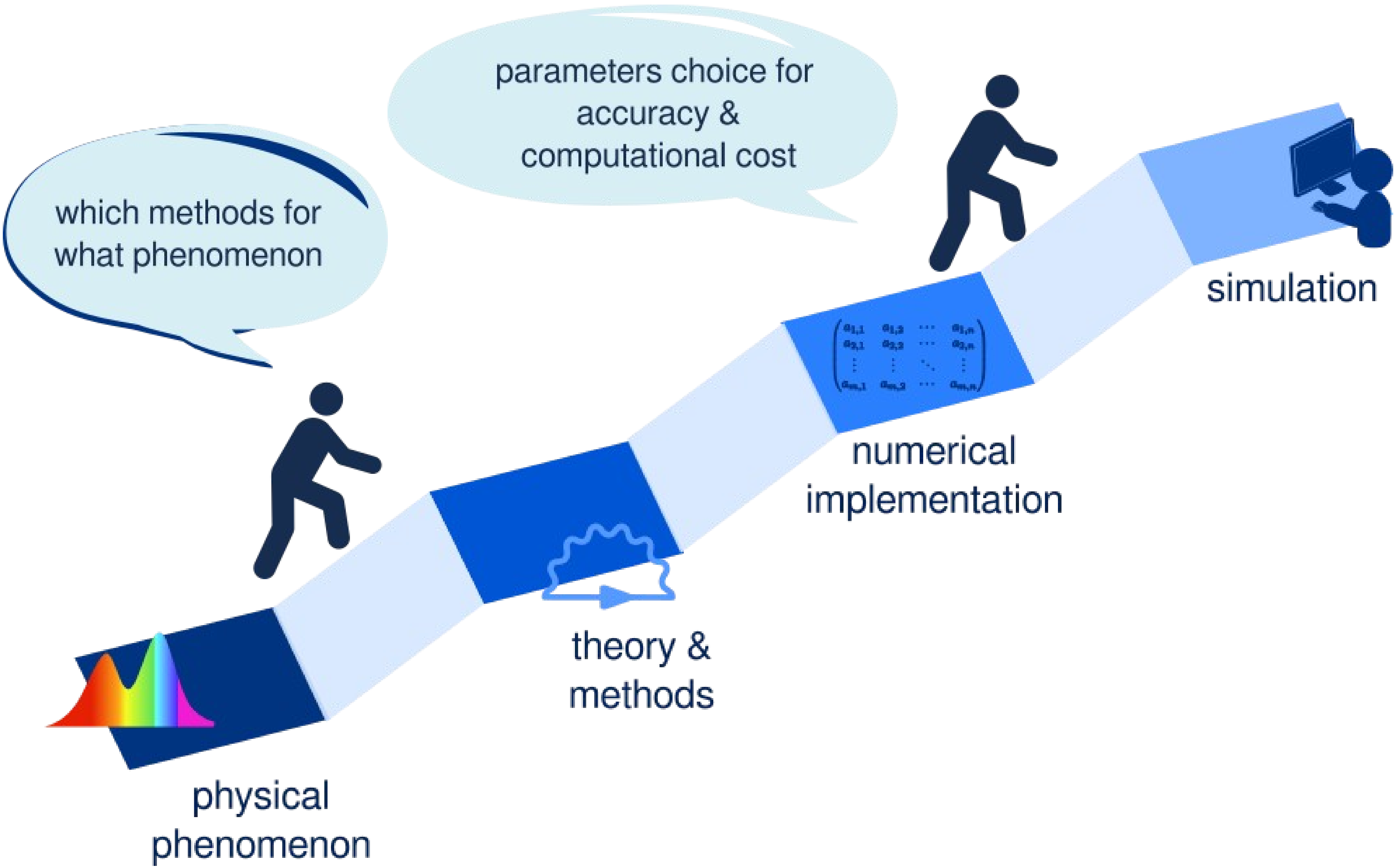
How can we answer the following questions...?

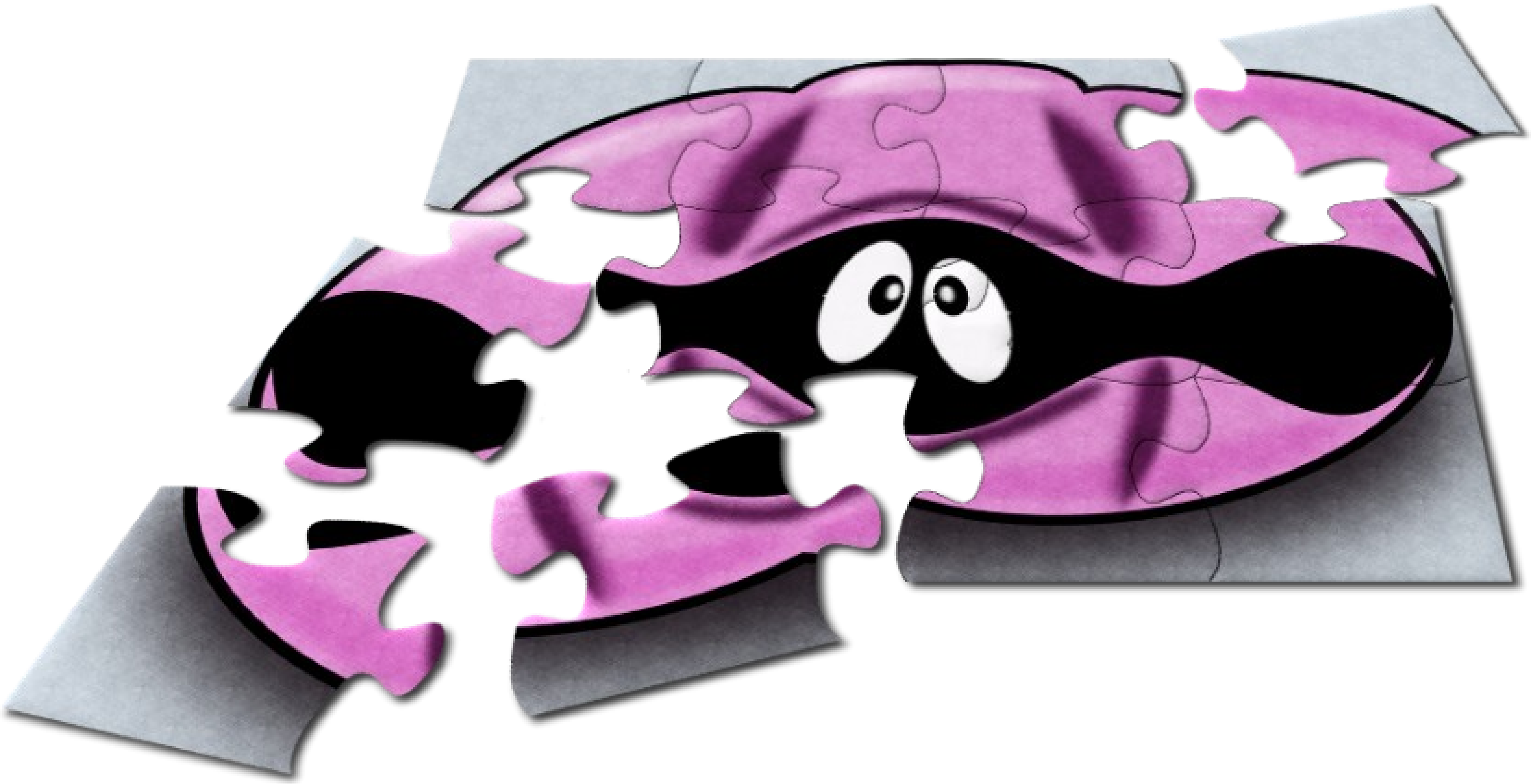


The first step is to 'read & study'



The Many-Body problem





the Yambo team

1. Many-body perturbation theory calculations using the yambo code
   Journal of Physics: Condensed Matter 31, 325902 (2019)
2. Yambo: an ab initio tool for excited state calculations
   Comp. Phys. Comm. 144, 180 (2009)

References & Material

Topic	Lecture	References
Exchange and Correlation Functionals	Talk	Refs
GW		Refs
Introduction to Spectroscopies	Talk	