

How To Do Simple Calculations With Quantum ESPRESSO



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I. About The Quantum ESPRESSO Distribution

Quantum ESPRESSO

- www.quantum-espresso.org



QUANTUM ESPRESSO

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25 May 2011 Version 4.3.1 of Quantum ESPRESSO is available for download.

05 May 2011
The first GPU-enabled beta release of Quantum ESPRESSO is available for download.

01 April 2011
The new release, v.4.3, of the Quantum ESPRESSO distribution is available for download.

13 July 2010
Bugfix release v.4.2.1 of the Quantum ESPRESSO distribution is available for download.

10 May 2010
A new version, v.4.2, of the Quantum ESPRESSO distribution is available for download.

12 April 2010
The final bugfix release, v.4.1.3, of the Quantum ESPRESSO distribution is available for download. This supersedes all previous 4.1.x releases.

Quantum ESPRESSO is an integrated suite of computer codes for electronic-structure calculations and materials modeling at the nanoscale. It is based on density-functional theory, plane waves, and pseudopotentials (both norm-conserving and ultrasoft).



What I cannot compute, I do not understand [adapted from Richard P. Feynman]

The Quantum ESPRESSO Software Distribution



The DEMOCRITOS center of Italian INFM is dedicated to atomistic simulations of materials, with a strong emphasis on the development of high-quality scientific software

Quantum ESPRESSO is the result of a DEMOCRITOS initiative, in collaboration with several other institutions (ICTP, CINECA Bologna, EPF Lausanne, Princeton University, MIT, Paris VI, Oxford, IJS Ljubljana,...)

Quantum ESPRESSO is a distribution of software for atomistic simulations based on electronic structure, using density-functional theory (DFT), a plane waves (PW) basis set and pseudopotentials (PP)

Quantum ESPRESSO stands for *Quantum opEn-Source Package for Research in Electronic Structure, Simulation, and Optimization*

P. Giannozzi

Why “Quantum ESPRESSO”?!



Trieste, Tommaseo (ph. G. Crozzoli)



Licence for Quantum ESPRESSO

Quantum ESPRESSO is distributed under the *GNU (Gnu's Not Unix) General Public License (GPL)*, probably the most common free-software license. Basically:

- The source code is available.
- You can do whatever you want with the sources, but if you distribute any derived work, you have to distribute under the GPL the sources of the derived work.

Advantages:

- Everybody – including commercial entities – can contribute.
- Nobody can “steal” the code and give nothing back to the community.

The most successful example is probably the Linux Kernel.

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Quantum ESPRESSO: Organization

The distribution is maintained as a single CVS (Concurrent Version System) tree. Available to everyone anytime via anonymous (read-only) access.

- *Web site:* <http://www.quantum-espresso.org>
- *Wiki:* http://www.quantum-espresso.org/index.php/Main_Page contains the updated documentation
- *Developers' portal:* <http://www.qe-forge.org>
integrated developer environment, open to external contributions

Mailing lists:

- *pw_users:* used by developers for announcements about Quantum ESPRESSO
- *pw_forum:* for general discussions (all subscribed users can post)

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Quantum ESPRESSO as a distribution

Quantum ESPRESSO aims at becoming a *distribution* of packages, rather than a single, monolithic, tightly integrated package. Main packages:

- PWscf: self-consistent electronic structure, structural relaxation, molecular dynamics
- CP/FPMD: variable-cell Car-Parrinello molecular dynamics

They share a common installation method, input format, PP format, data output format, large parts of the basic code. More packages:

- PHonon: linear-response calculations (phonons, dielectric properties)
- PostProc: graphical and postprocessing utilities (density of states, STM, etc.)
- atomic: pseudopotential generation code
- PWGui: a Graphical User Interface for production of input files

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Quantum ESPRESSO as a distribution

OTHER PACKAGES

WANNIER90: Maximally localized Wannier functions

Pwcond: Ballistic conductance

WanT: Coherent Transport from Maximally Localized Wannier Functions

Xspectra: Calculation of x-ray near edge absorption spectra

GIPAW: EPR and NMR Chemical Shifts

Coming Soon:

GW: GW Band Structure with Ultralocalized Wannier Fns.

TD-DFT: Time-Dependent Density Functional Pert. Theory

What Can Quantum ESPRESSO Do?

- Both Γ point and k-point calculations.
- Both insulators and metals, with smearing.
- Any crystal structure or supercell form.
- Norm conserving pseudopotentials, ultrasoft PPs, PAW.
- LDA, GGA, DFT+U, hybrid functionals, exact exchange, meta GGA, van der Waals corrected functionals.
- Spin polarized calculations, non-collinear magnetism, spin-orbit interactions.
- Nudged elastic band to find saddle points.



II. Doing a “Total Energy” Calculation with the PWscf Package of QE: The SCF Loop

The Kohn-Sham problem

- Want to solve the Kohn-Sham equations:

$$\left[-\frac{1}{2} \nabla^2 + V_{nuc}(\mathbf{r}) + V_H[n(\mathbf{r})] + V_{XC}[n(\mathbf{r})] \right] \psi_i(\mathbf{r}) = \varepsilon_i \psi_i(\mathbf{r})$$

H

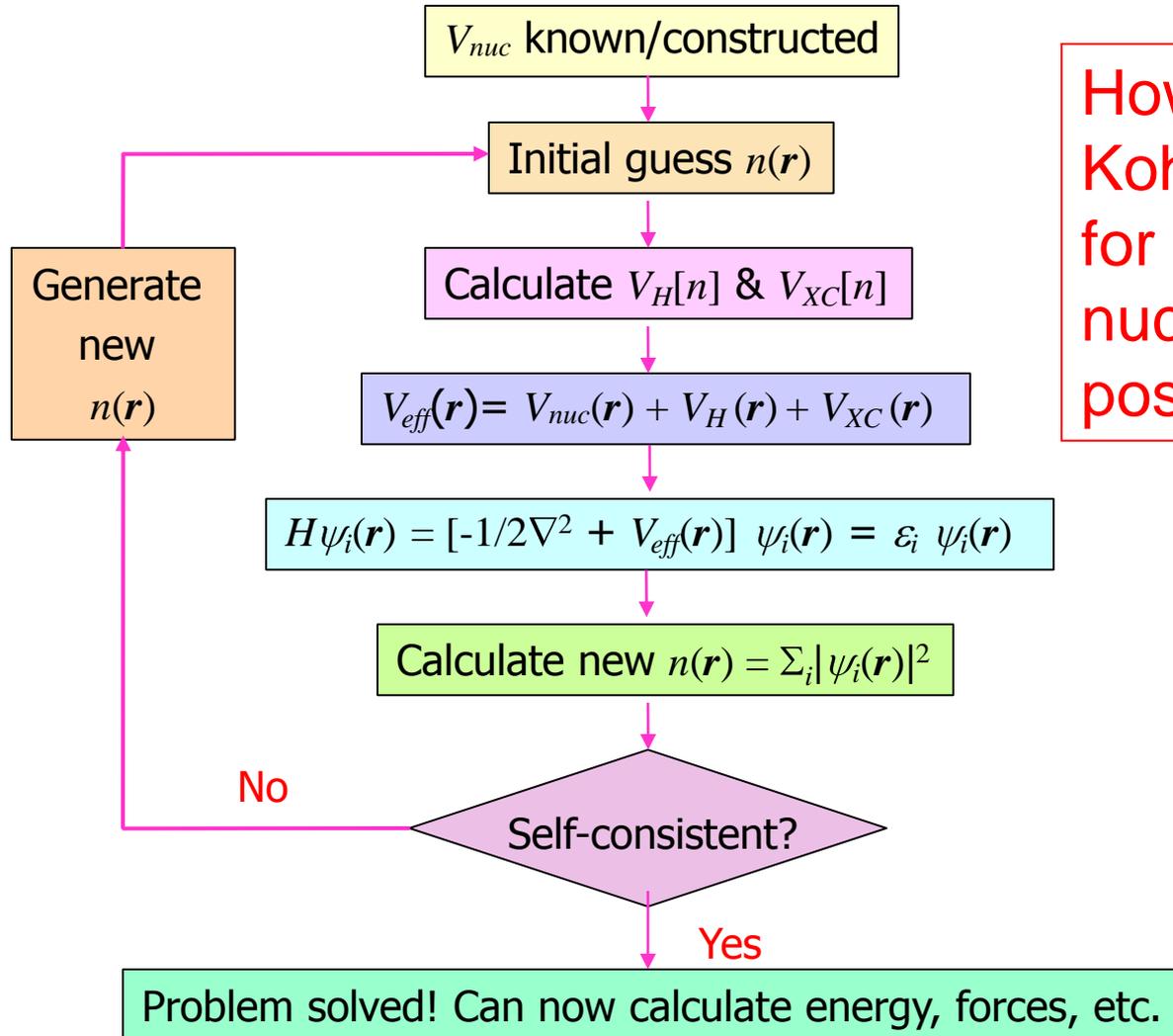
- Note that **self-consistent solution** necessary, as H depends on solution:

$$\{\psi_i\} \rightarrow n(r) \rightarrow H$$

- Convention:

$$e = \hbar = m_e = 1$$

Self-consistent Iterative Solution



How to solve the Kohn-Sham eqns. for a set of fixed nuclear (ionic) positions.

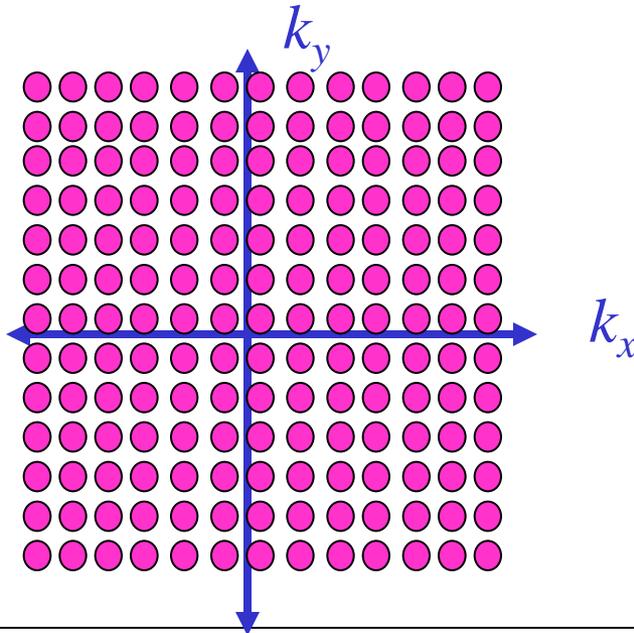
Plane Waves & Periodic Systems

- For a periodic system:

$$\psi_{\mathbf{k}}(\mathbf{r}) = \frac{1}{\Omega} \sum_{\mathbf{G}} c_{\mathbf{k},\mathbf{G}} e^{i(\mathbf{k}+\mathbf{G})\cdot\mathbf{r}}$$

where \mathbf{G} = reciprocal lattice vector

- The **plane waves** that appear in this expansion can be represented as a grid in k-space:



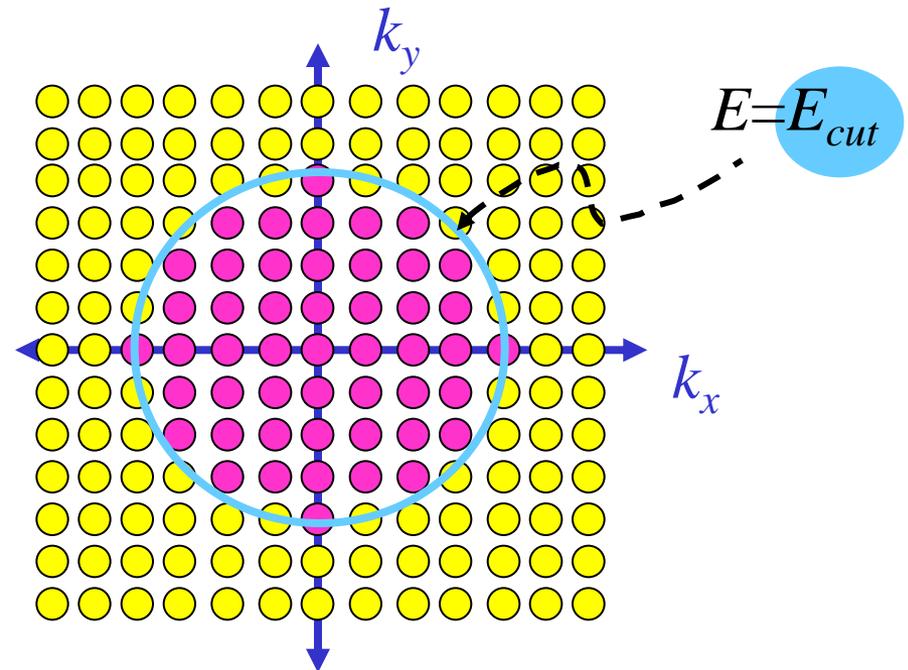
- Only true for periodic systems that grid is discrete.
- In principle, still need **infinite number of plane waves**.

Truncating the Plane Wave Expansion

- In practice, the contribution from higher Fourier components (large $|\mathbf{k}+\mathbf{G}|$) is small.
- So truncate the expansion at some value of $|\mathbf{k}+\mathbf{G}|$.
- Traditional to express this cut-off in energy units:

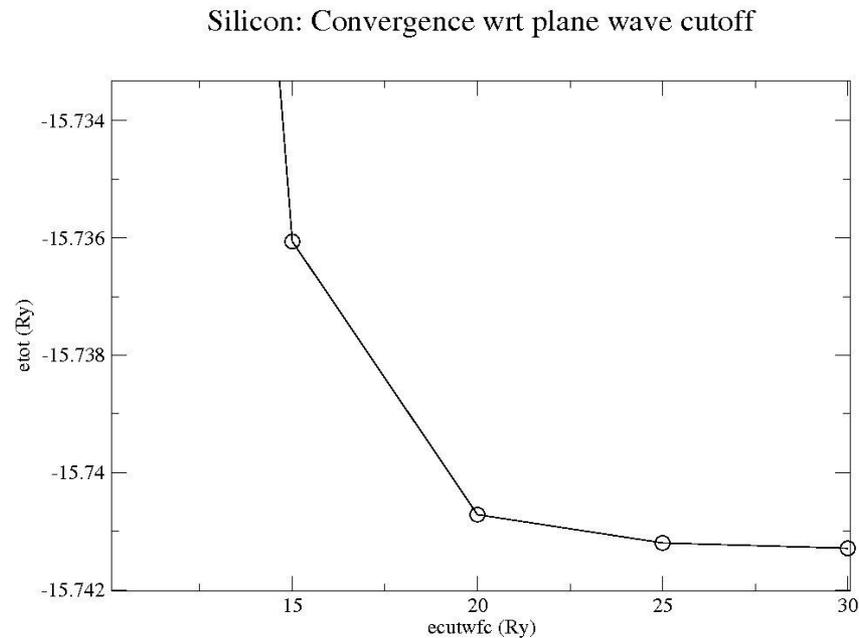
$$\frac{\hbar^2 |\mathbf{k} + \mathbf{G}|^2}{2m} \leq E_{cut}$$

Input parameter **ecutwfc**



Checking Convergence wrt $ecutwfc$

- Must always check.
- Monotonic (variational).



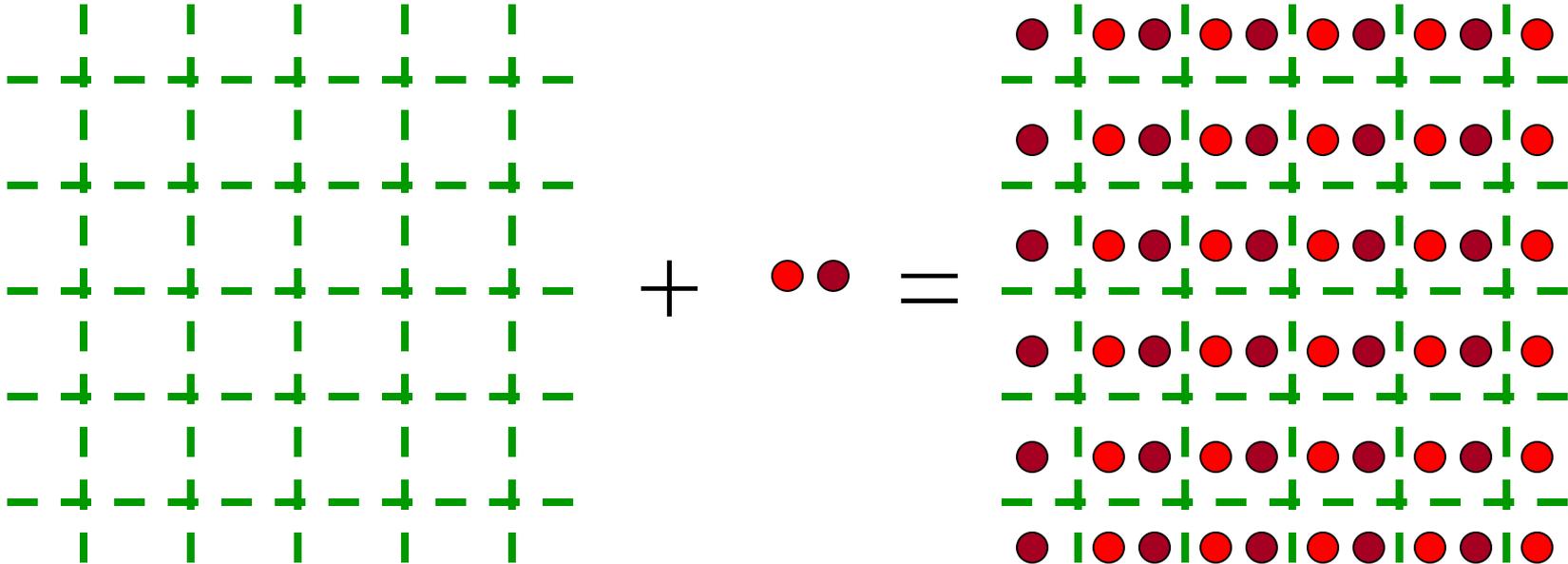
Step 0: Defining the (periodic) system



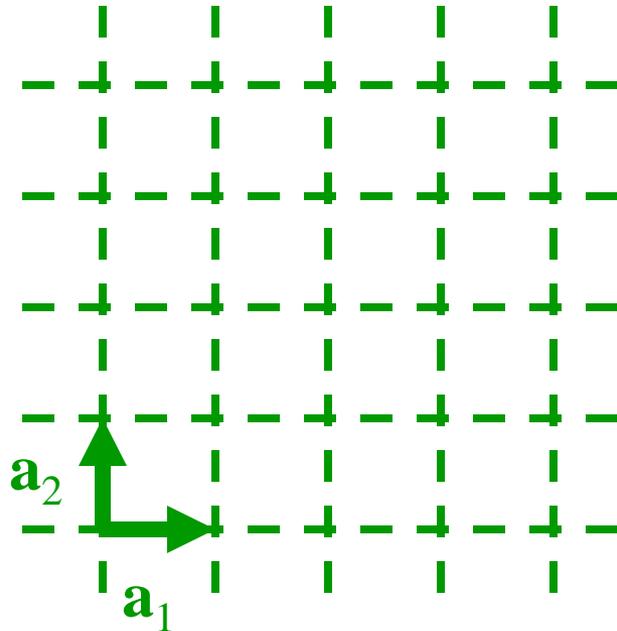
Namelist '**SYSTEM**'

How to Specify the System

- All periodic systems can be specified by a **Bravais Lattice** and an **atomic basis**.



How to Specify the Bravais Lattice / Unit Cell



Input parameter **ibrav**

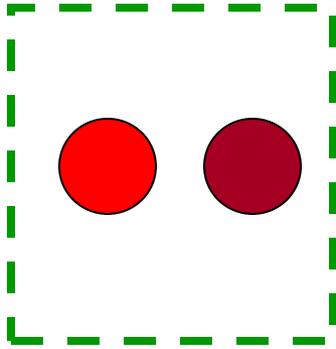
- Gives the type of **Bravais lattice** (SC, BCC, Hex, etc.)

Input parameters { **celldm(i)** }

- Give the lengths [& directions, if necessary] of the lattice vectors \mathbf{a}_1 , \mathbf{a}_2 , \mathbf{a}_3

- Note that one can choose a non-primitive unit cell (e.g., 4 atom SC cell for FCC structure).

Atoms Within Unit Cell – How many, where?



Input parameter **nat**

- Number of atoms in the unit cell

Input parameter **ntyp**

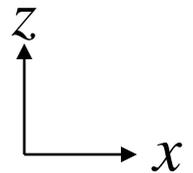
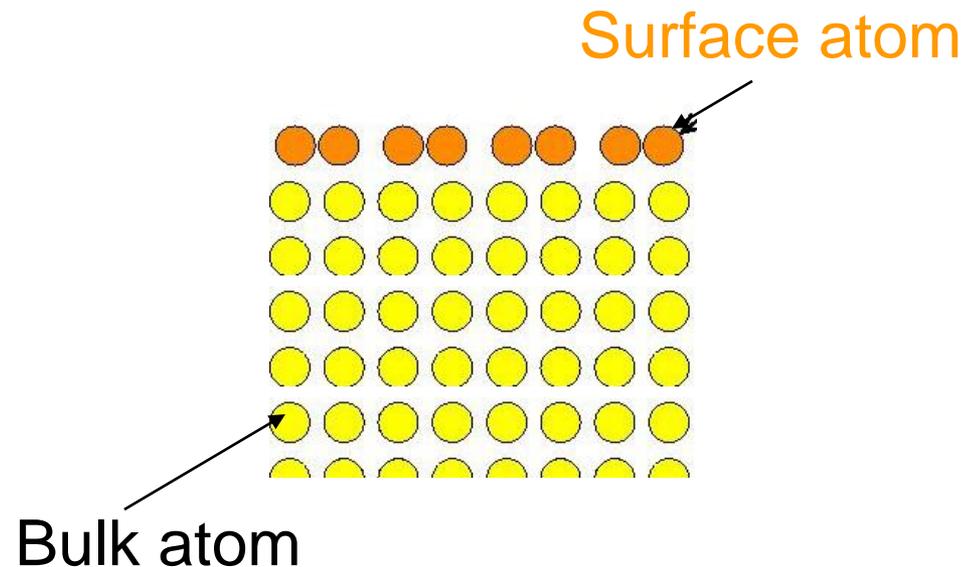
- Number of types of atoms

FIELD **ATOMIC_POSITIONS**

- Initial positions of atoms (may vary when “**relax**” done).
- Can choose to give in units of lattice vectors (“**crystal**”) or in Cartesian units (“**alat**” or “**bohr**” or “**angstrom**”)

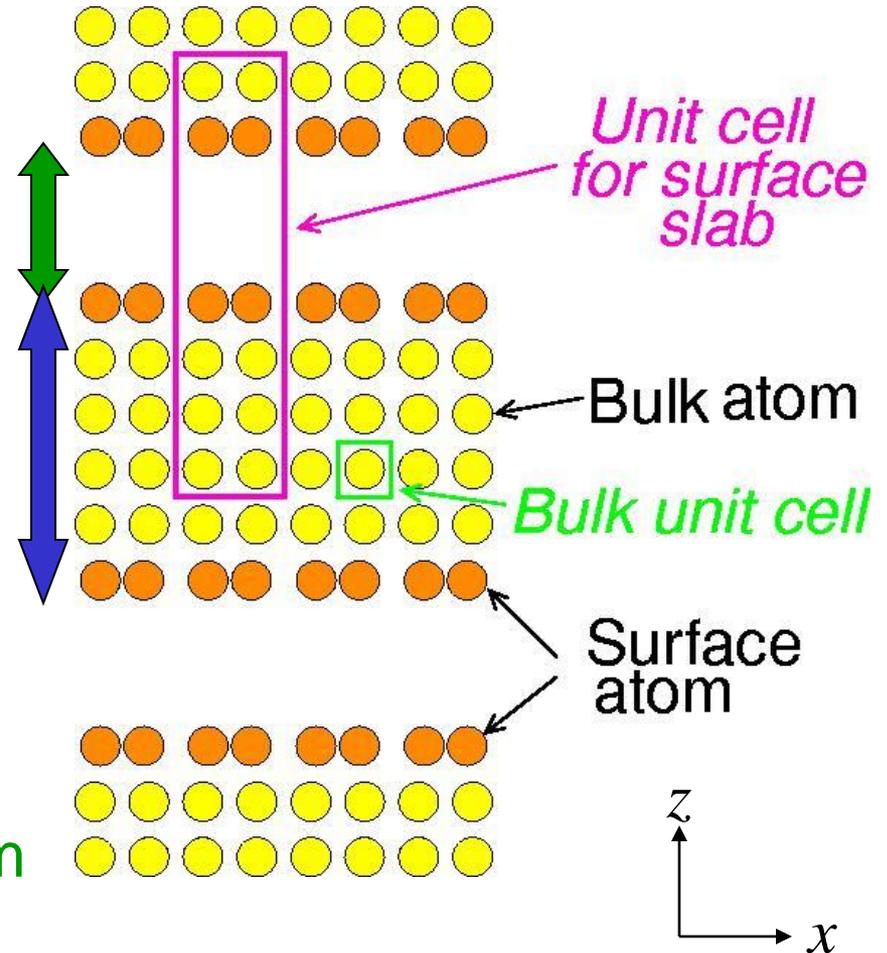
What if the system is not periodic?

- Example 1: Want to study properties of a system with a **surface**.
- Presence of surface \Rightarrow No periodicity along z .



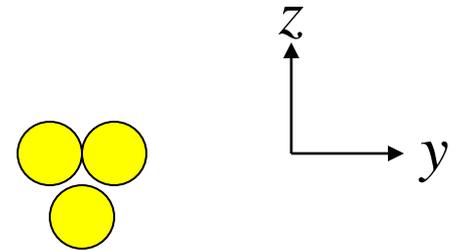
What if the system is not periodic?

- Example 1: Want to study properties of a system with a **surface**.
- Presence of surface \Rightarrow No periodicity along z .
- Use a **supercell**: **artificial periodicity along z** by repeating slabs separated by **vacuum**.
- Have to check convergence w.r.t. **slab thickness** & **vacuum thickness**.



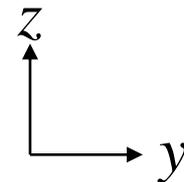
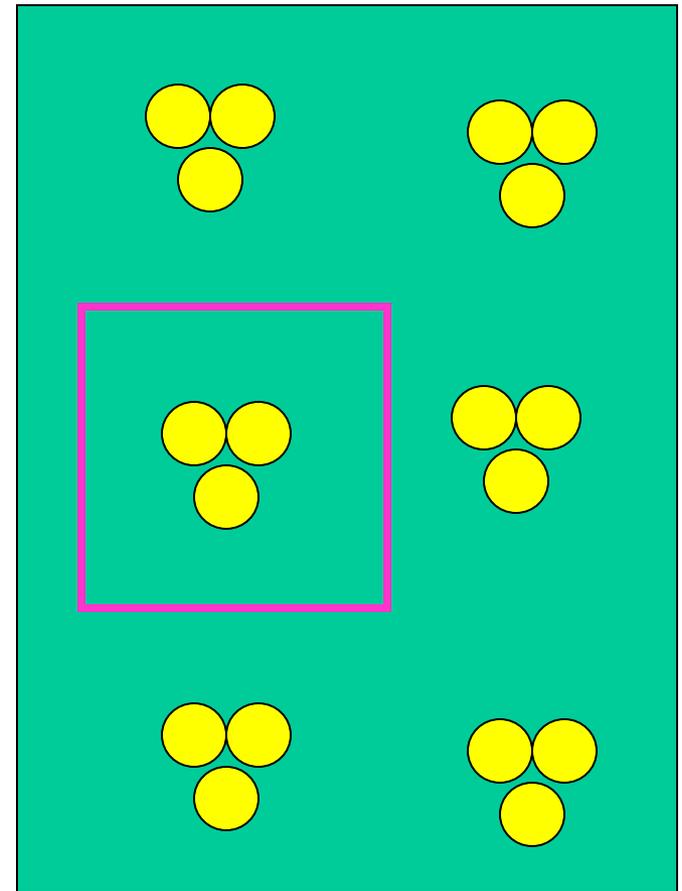
What if the system is not periodic?

- Example 2: Want to study properties of a nanowire.
- Example 3: Want to study properties of a cluster



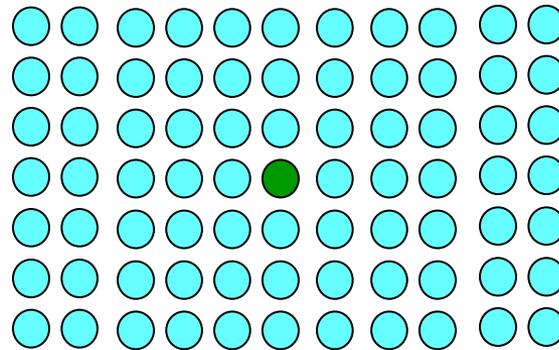
What if the system is not periodic?

- Example 2: Want to study properties of a nanowire \Rightarrow introduce **artificial periodicity along y & z** .
- Example 3: Want to study properties of a cluster \Rightarrow introduce **artificial periodicity along x , y & z** .



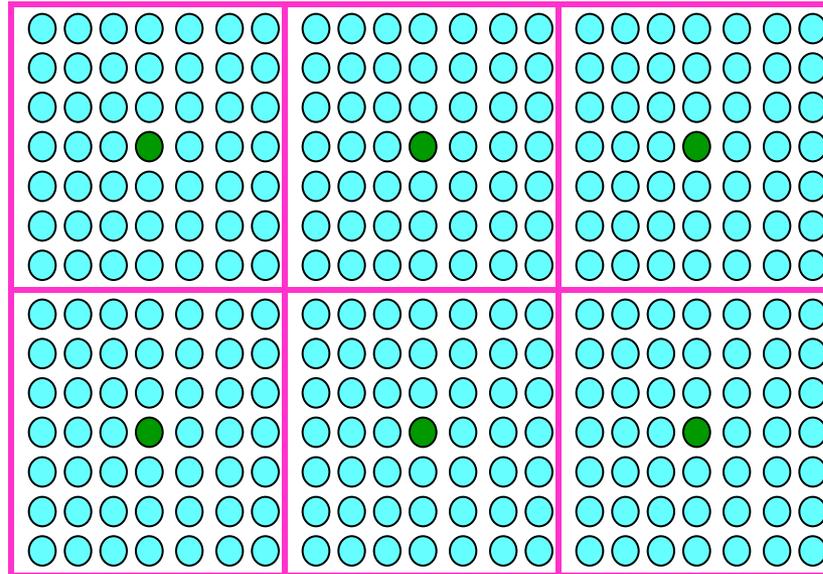
What if the system is not periodic?

- Example 4: Want to study a system with a defect, e.g., a **vacancy or impurity**:



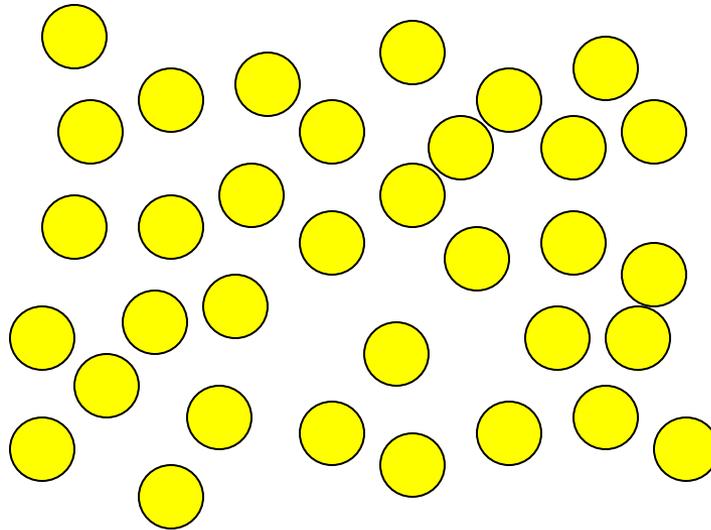
What if the system is not periodic?

- Example 4: Want to study a system with a defect, e.g., a **vacancy or impurity**:



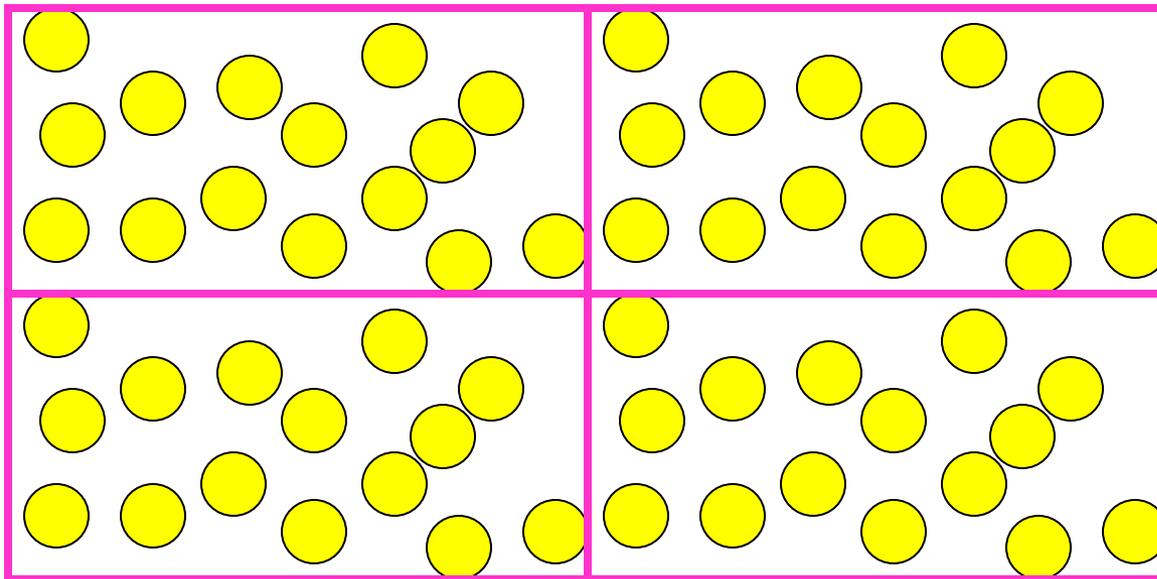
What if the system is not periodic?

- Example 5: Want to study an amorphous or quasicrystalline system.



What if the system is not periodic?

- Example 5: Want to study an amorphous or quasicrystalline system: approximate by a periodic system (with large **unit cell**).



Artificially Periodic Systems \Rightarrow Large Unit Cells

- Note: In all these cases, to minimize the effects of the artificially introduced periodicity, need a large unit cell.



- Long $\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3$ (primitive lattice vectors)

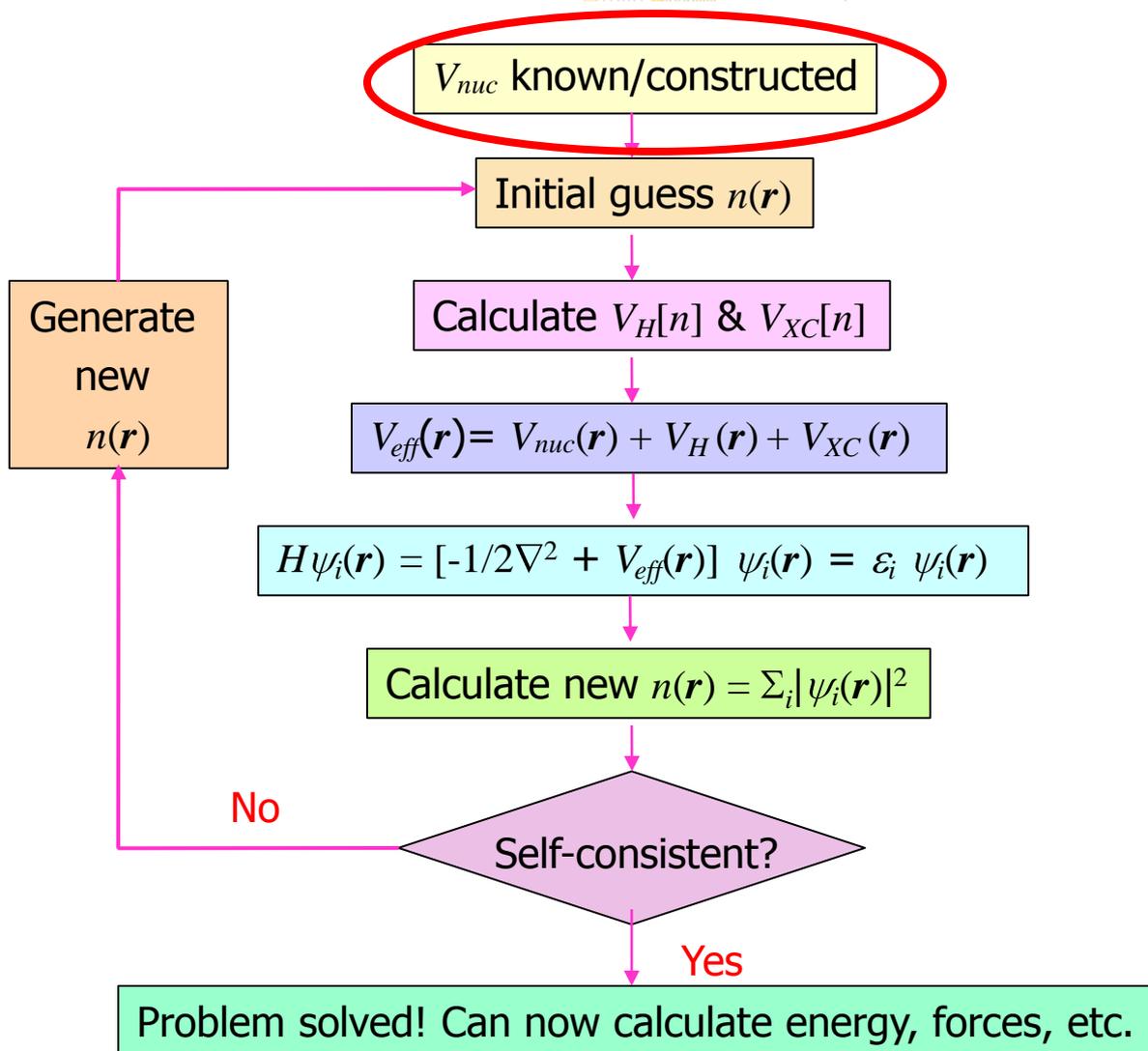


- Short $\mathbf{b}_1, \mathbf{b}_2, \mathbf{b}_3$ (primitive reciprocal lattice vectors)



- Many \mathbf{G} 's will fall within E_{cut} sphere!

Step 1: Obtaining V_{nuc}



Nuclear Potential

- Electrons experience a **Coulomb potential** due to the nuclei.
- This has a known and simple form:

$$V_{nuc} = -\frac{Z}{r}$$

- But this leads to computational problems!

Problem for Plane-Wave Basis

Core wavefunctions:
sharply peaked near
nucleus.

Valence wavefunctions:
lots of wiggles near
nucleus.

High Fourier components present

i.e., need large E_{cut} ☹️

Solutions for Plane-Wave Basis

Core wavefunctions:
sharply peaked near
nucleus.

Valence wavefunctions:
lots of wiggles near
nucleus.

High Fourier components present

i.e., need large E_{cut} ☹️

Don't solve for the
core electrons!

Remove wiggles from
valence electrons.

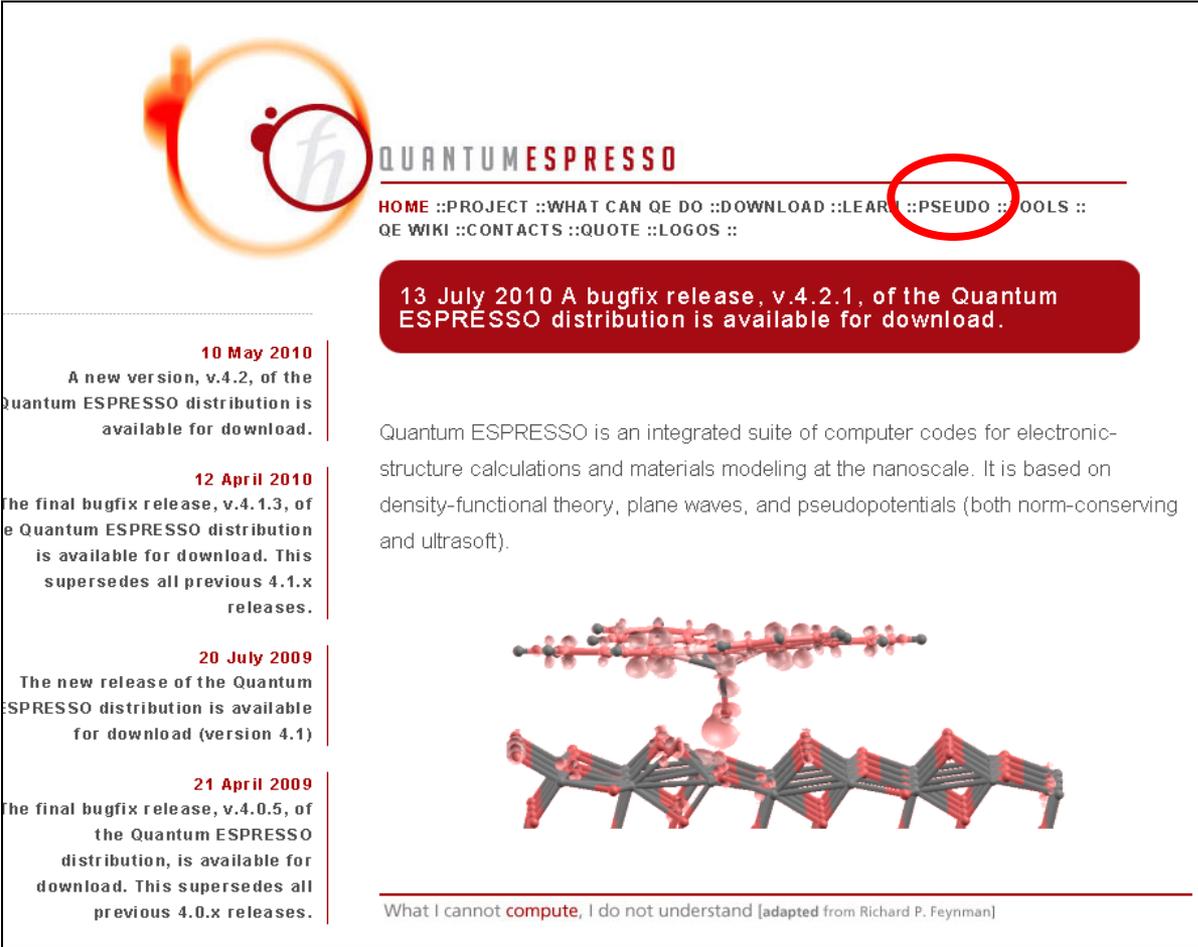
Pseudopotentials



- Replace nuclear potential by **pseudopotential**
- This is a numerical trick that solves these problems
- There are different kinds of pseudopotentials (Norm conserving pseudopotentials, ultrasoft pseudopotentials, etc.)
- Which kind you use depends on the element.

Pseudopotentials for Quantum Espresso - 1

- Go to <http://www.quantum-espresso.org>; Click on “PSEUDO”



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13 July 2010 A bugfix release, v.4.2.1, of the Quantum ESPRESSO distribution is available for download.

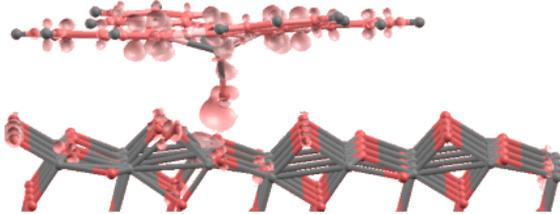
10 May 2010
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12 April 2010
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20 July 2009
The new release of the Quantum ESPRESSO distribution is available for download (version 4.1)

21 April 2009
The final bugfix release, v.4.0.5, of the Quantum ESPRESSO distribution, is available for download. This supersedes all previous 4.0.x releases.

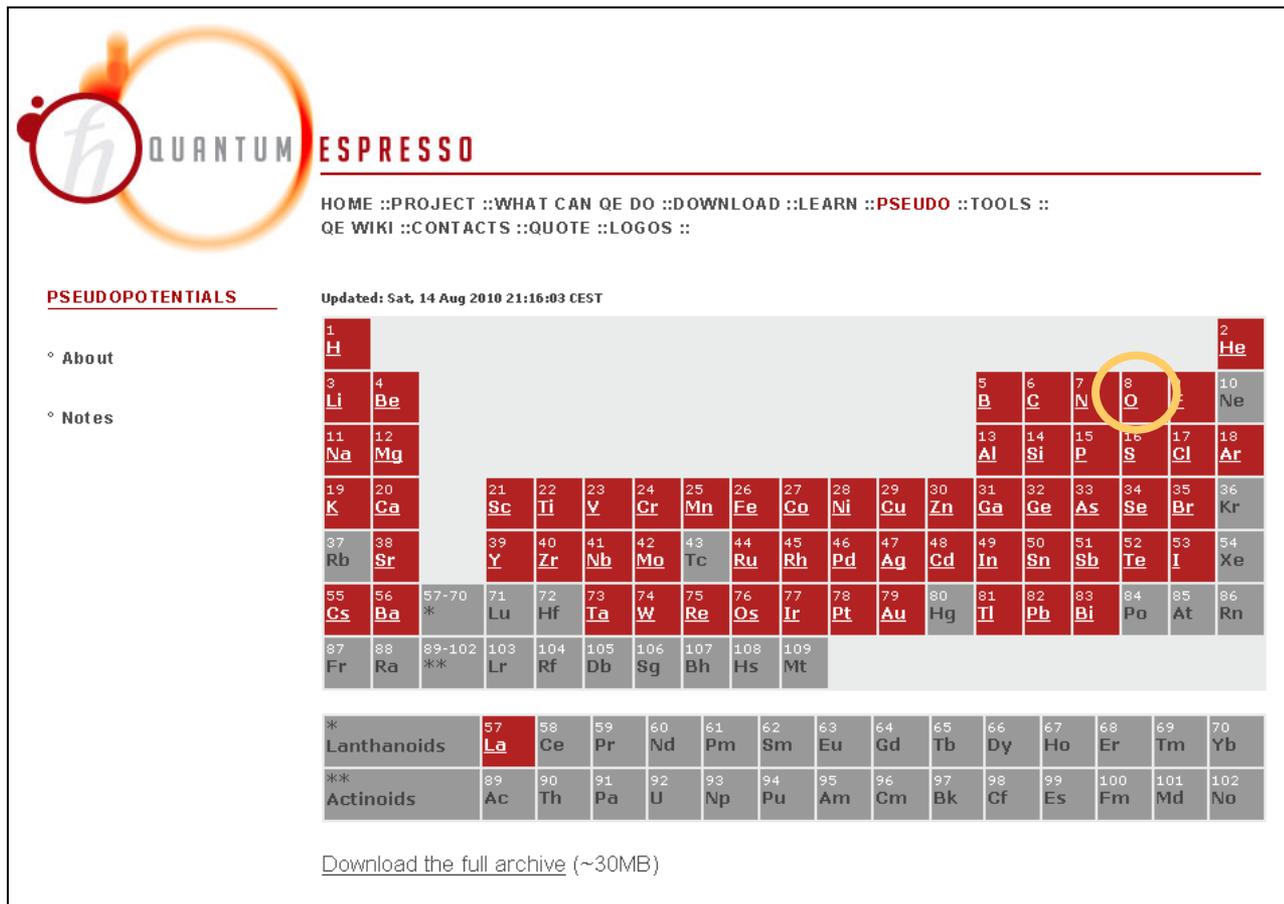
Quantum ESPRESSO is an integrated suite of computer codes for electronic-structure calculations and materials modeling at the nanoscale. It is based on density-functional theory, plane waves, and pseudopotentials (both norm-conserving and ultrasoft).



What I cannot **compute**, I do not understand [adapted from Richard P. Feynman]

Pseudopotentials for Quantum Espresso - 2

- Click on element for which pseudopotential wanted.



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PSEUDOPOTENTIALS

Updated: Sat, 14 Aug 2010 21:16:03 CEST

◦ About
◦ Notes

1 H																	2 He	
3 Li	4 Be											5 B	6 C	7 N	8 O	9 F	10 Ne	
11 Na	12 Mg											13 Al	14 Si	15 P	16 S	17 Cl	18 Ar	
19 K	20 Ca	21 Sc	22 Ti	23 V	24 Cr	25 Mn	26 Fe	27 Co	28 Ni	29 Cu	30 Zn	31 Ga	32 Ge	33 As	34 Se	35 Br	36 Kr	
37 Rb	38 Sr	39 Y	40 Zr	41 Nb	42 Mo	43 Tc	44 Ru	45 Rh	46 Pd	47 Ag	48 Cd	49 In	50 Sn	51 Sb	52 Te	53 I	54 Xe	
55 Cs	56 Ba	57-70 *	71 Lu	72 Hf	73 Ta	74 W	75 Re	76 Os	77 Ir	78 Pt	79 Au	80 Hg	81 Tl	82 Pb	83 Bi	84 Po	85 At	86 Rn
87 Fr	88 Ra	89-102 **	103 Lr	104 Rf	105 Db	106 Sg	107 Bh	108 Hs	109 Mt									
* Lanthanoids			57 La	58 Ce	59 Pr	60 Nd	61 Pm	62 Sm	63 Eu	64 Gd	65 Tb	66 Dy	67 Ho	68 Er	69 Tm	70 Yb		
** Actinoids			89 Ac	90 Th	91 Pa	92 U	93 Np	94 Pu	95 Am	96 Cm	97 Bk	98 Cf	99 Es	100 Fm	101 Md	102 No		

[Download the full archive \(~30MB\)](#)

Pseudopotentials for Quantum-ESPRESSO

Name: **Oxygen**

Symbol: **O**

Atomic number: **8**

Atomic configuration: **[He] 2s2 2p4**

Atomic mass: **15.9994 (3)**

Available pseudopotentials:

O.blyp-mt.UPF (details)

Becke-Lee-Yang-Parr (BLYP) exch-corr
Martins-Troullier

O.pbe-rrkjus.UPF (details)

Perdew-Burke-Ernzerhof (PBE) exch-corr
Rabe Rappe Kaxiras Joannopoulos (ultrasoft)

O.pbe-van_bm.UPF (details)

Perdew-Burke-Ernzerhof (PBE) exch-corr
Vanderbilt ultrasoft
author: bm

O.pz-mt.UPF (details)

Perdew-Zunger (LDA) exch-corr
Martins-Troullier

O.pz-rrkjus.UPF (details)

Perdew-Zunger (LDA) exch-corr
Rabe Rappe Kaxiras Joannopoulos (ultrasoft)

O.blyp-van_ak.UPF (details)

Becke-Lee-Yang-Parr (BLYP) exch-corr
Vanderbilt ultrasoft
author: ak

Pseudopotential's name
gives information about :

- type of exchange-correlation functional
- type of pseudopotential
- e.g.:

O.pbe-rrkjus.UPF (details)

Perdew-Burke-Ernzerhof (PBE) exch-corr
Rabe Rappe Kaxiras Joannopoulos (ultrasoft)

Element & V_{ion} for Quantum-ESPRESSO

e.g, for calculation on BaTiO₃:

ATOMIC_SPECIES

```
Ba 137.327 Ba.pbe-nsp-van.UPF
```

```
Ti 47.867 Ti.pbe-sp-van_ak.UPF
```

```
O 15.999 O.pbe-van_ak.UPF
```

- **ecutwfc**, **ecutrho** depend on type of pseudopotentials used (should test).
- When using ultrasoft pseudopotentials, set **ecutrho = 8-12 × ecutwfc !!**

Element & V_{ion} for Quantum-ESPRESSO

- Should have same exchange-correlation functional for all pseudopotentials.

input

```
diagonalization = cg, mixing_mode
mixing_beta = 0.7, conv_thr = 1.0
/
ATOMIC_SPECIES
Fe 55.85 Fe pz-nd-rrkjus.UPF
Co 58.93 Co pbe-nd-rrkjus.UPF
ATOMIC_POSITIONS (crystal)
Fe 0.00 0.00 0.00
```

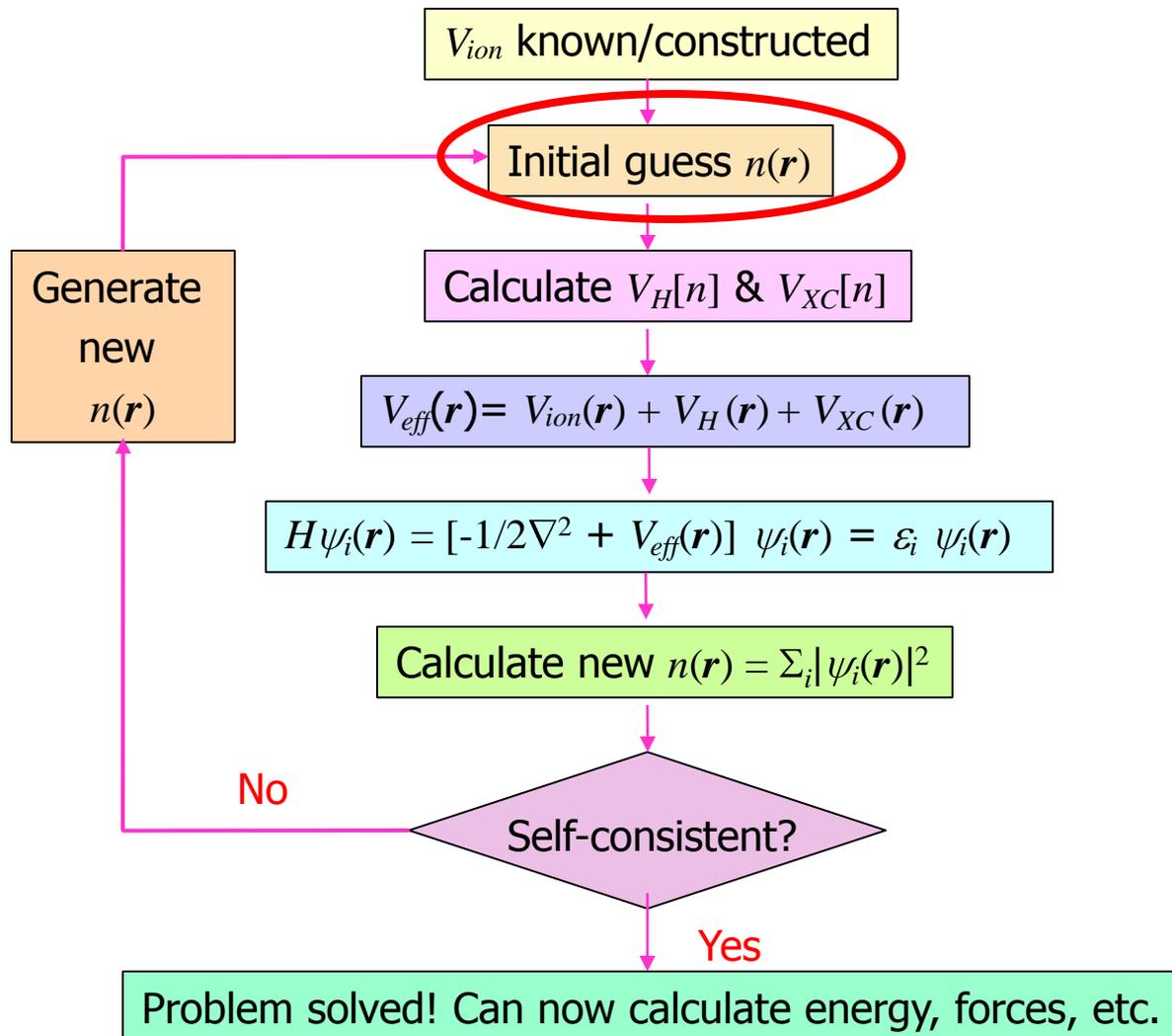
oops!

output

```
Max angular momentum in pseudopotentials
XXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXX
from readpp : error #          2
inconsistent DFT read
XXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXX

stopping ..█
```

Step 2: Initial Guess for $n(\mathbf{r})$



Starting Wavefunctions

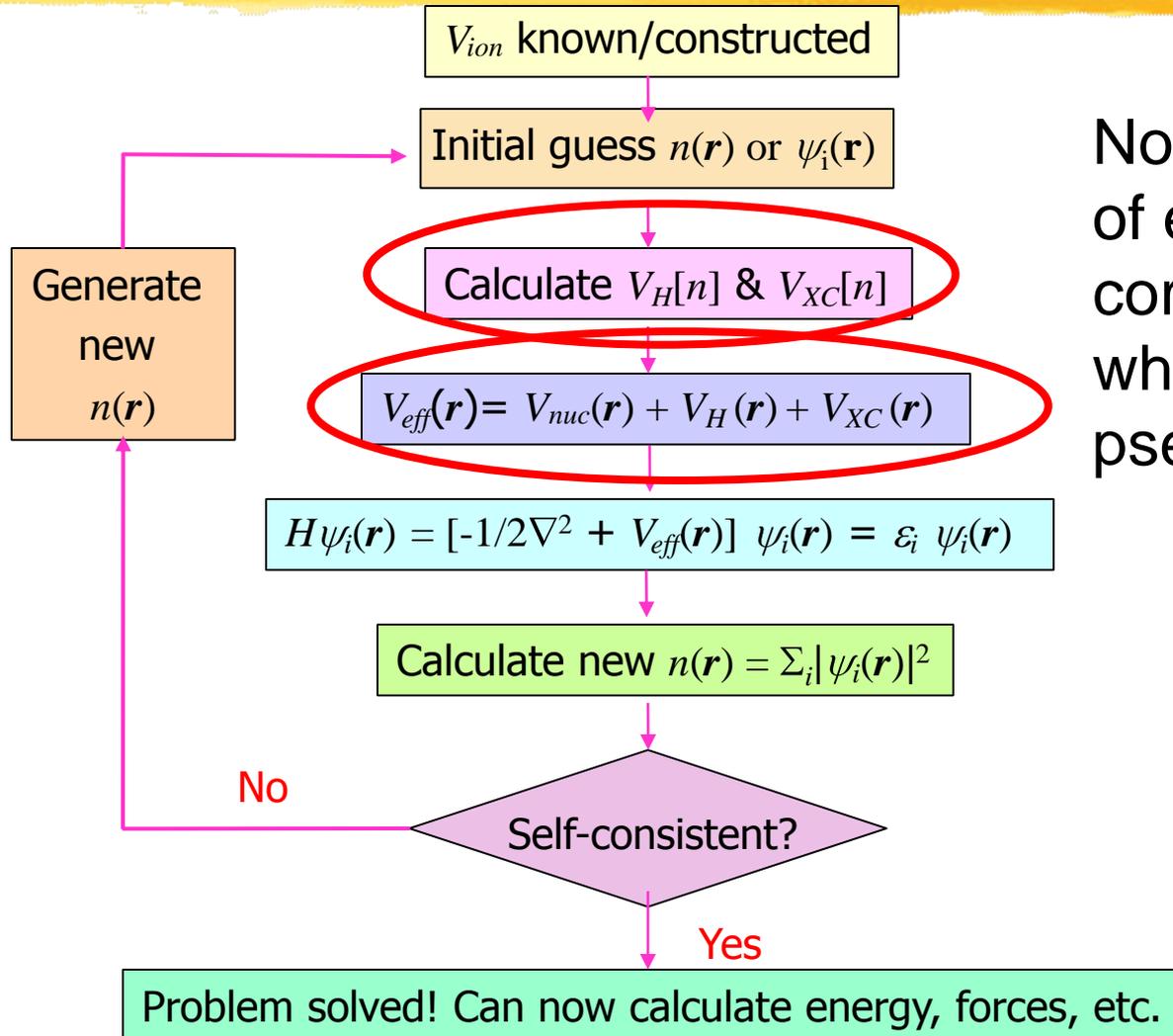
The closer your starting wavefunction is to the true wavefunction (which, of course, is something you don't necessarily know to start with!), the fewer the scf iterations needed.

```
startingwfc 'atomic'  
            'random'  
            'file'
```

Superposition of atomic orbitals

“The beginning is the most important part of the work” - Plato

Steps 3 & 4: Effective Potential



Note that type of exchange-correlation chosen while specifying pseudopotential



Exchange-Correlation Potential

- $V_{XC} \equiv \delta E_{XC} / \delta n$ contains all the many-body information.
- Known [numerically, from Quantum Monte Carlo ; various analytical approximations] for **homogeneous electron gas**.

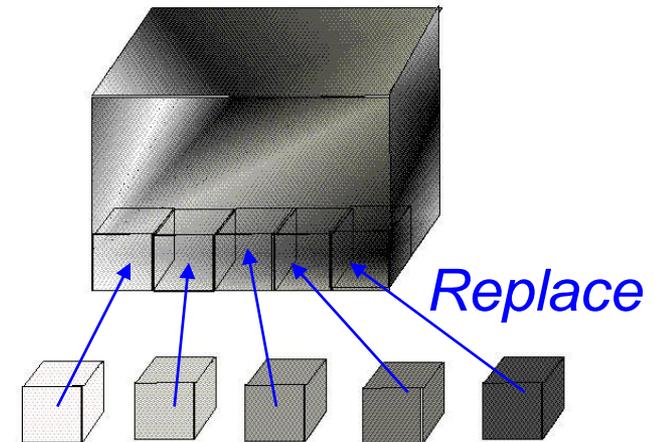
- **Local Density Approximation:**

$$E_{xc}[n] = \int n(\mathbf{r}) V_{xc}^{\text{HOM}}[n(\mathbf{r})] d\mathbf{r}$$

-surprisingly successful!

pz

(in name of pseudopotential)

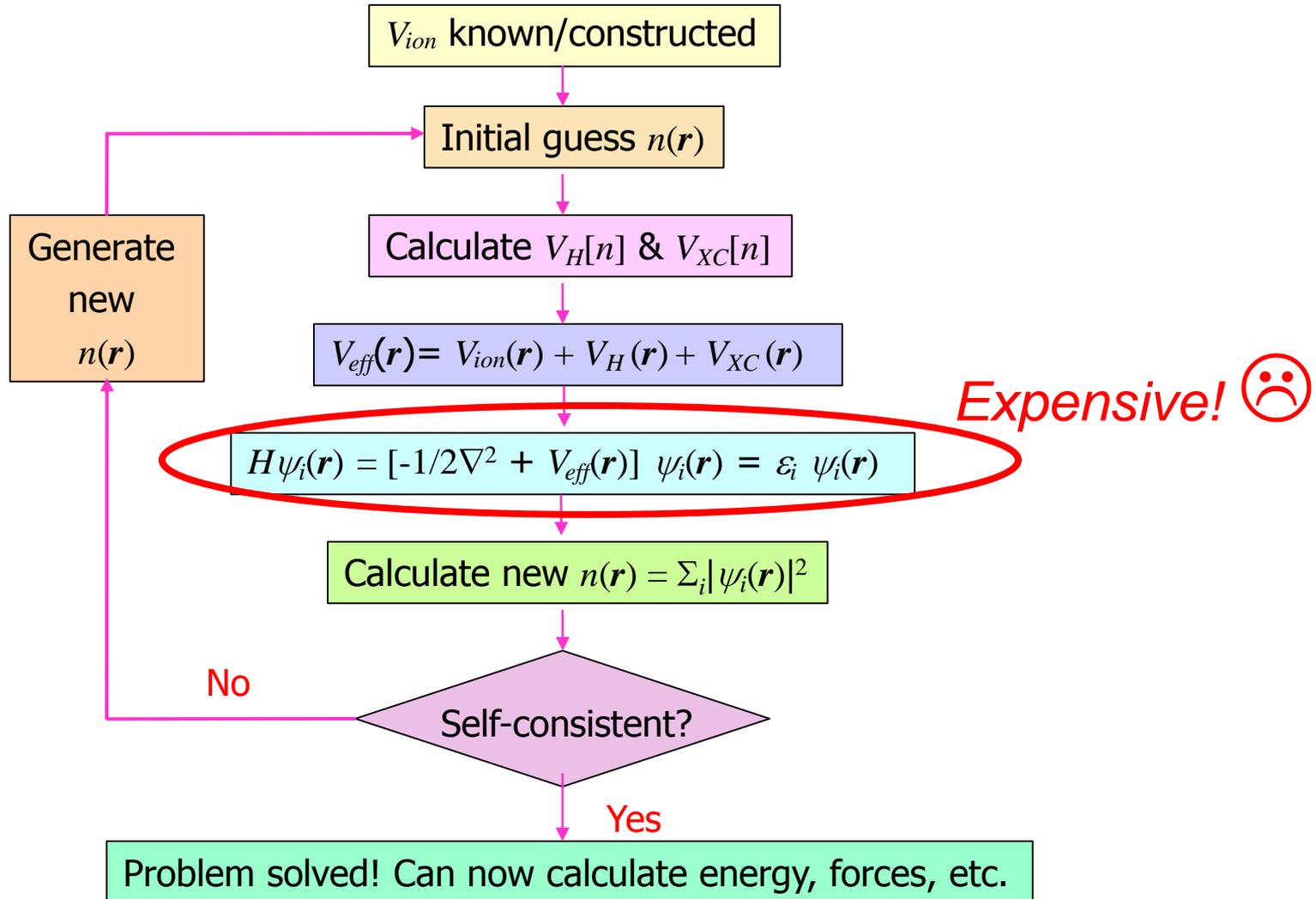


- **Generalized Gradient Approximation(s):** Include terms involving gradients of $n(\mathbf{r})$

pw91, pbe

(in name of pseudopotential)

Step 5: Diagonalization



Diagonalization

- Need to diagonalize a matrix of size $N_{PW} \times N_{PW}$
- $N_{PW} \gg N_b$ = number of bands required = $N_e/2$ or a little more (for metals).
- OK to obtain lowest few eigenvalues.
- Exact diagonalization is expensive!
- Use **iterative diagonalizers** that recast diagonalization as a minimization problem.

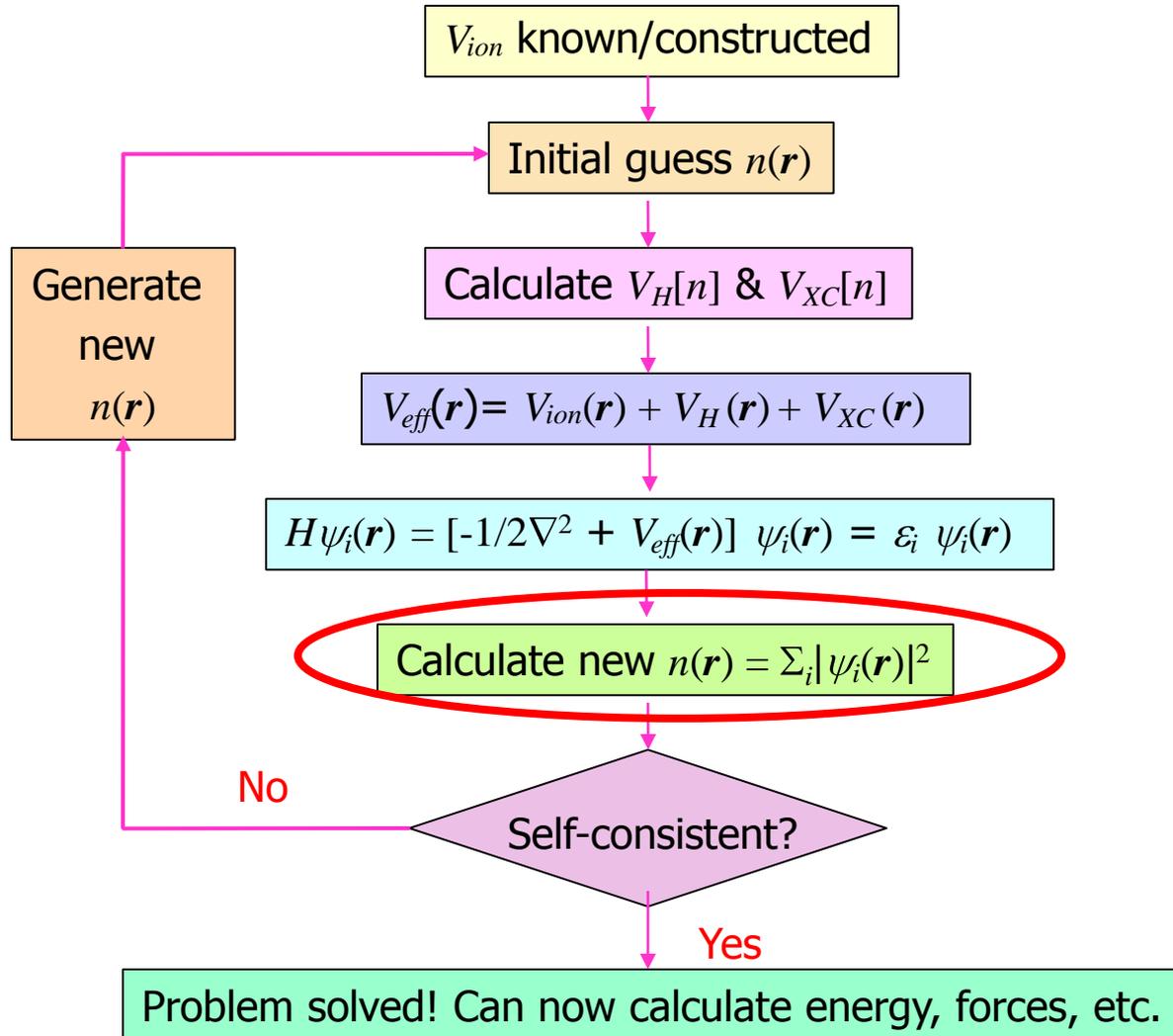
Input parameter **diagonalization**

-which algorithm used for iterative diagonalization

Input parameter **nbnd**

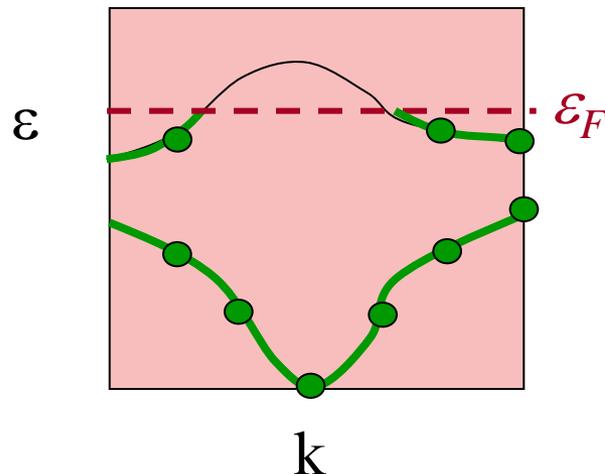
*-how many eigenvalues computed
for metals, choose depending on value of **degauss***

Step 6: New Charge Density



Brillouin Zone Sums

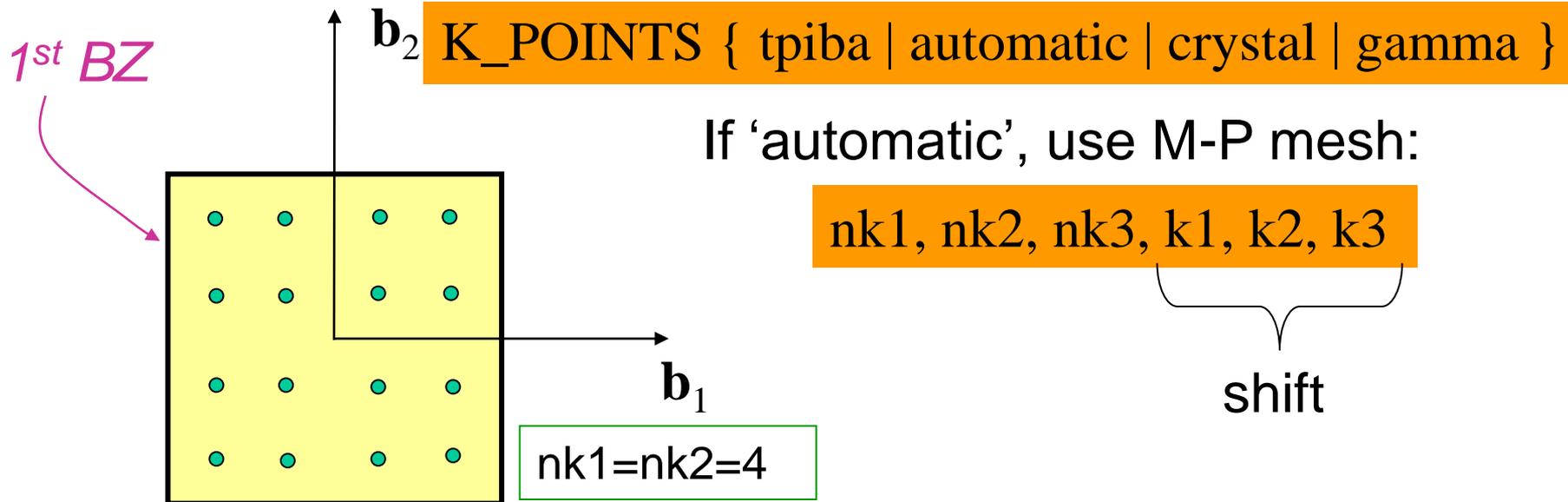
- Many quantities (e.g., n , E_{tot}) involve sums over \mathbf{k} .
- In principle, need infinite number of \mathbf{k} 's.
- In practice, sum over a finite number: BZ “Sampling”.
- Number needed depends on band structure.
- Typically need more \mathbf{k} 's for metals.
- Need to test convergence wrt k-point sampling.



$$\langle P \rangle = \frac{1}{N_{\mathbf{k}}} \sum_{\mathbf{k} \in BZ} P(\mathbf{k}) w_{\mathbf{k}}$$

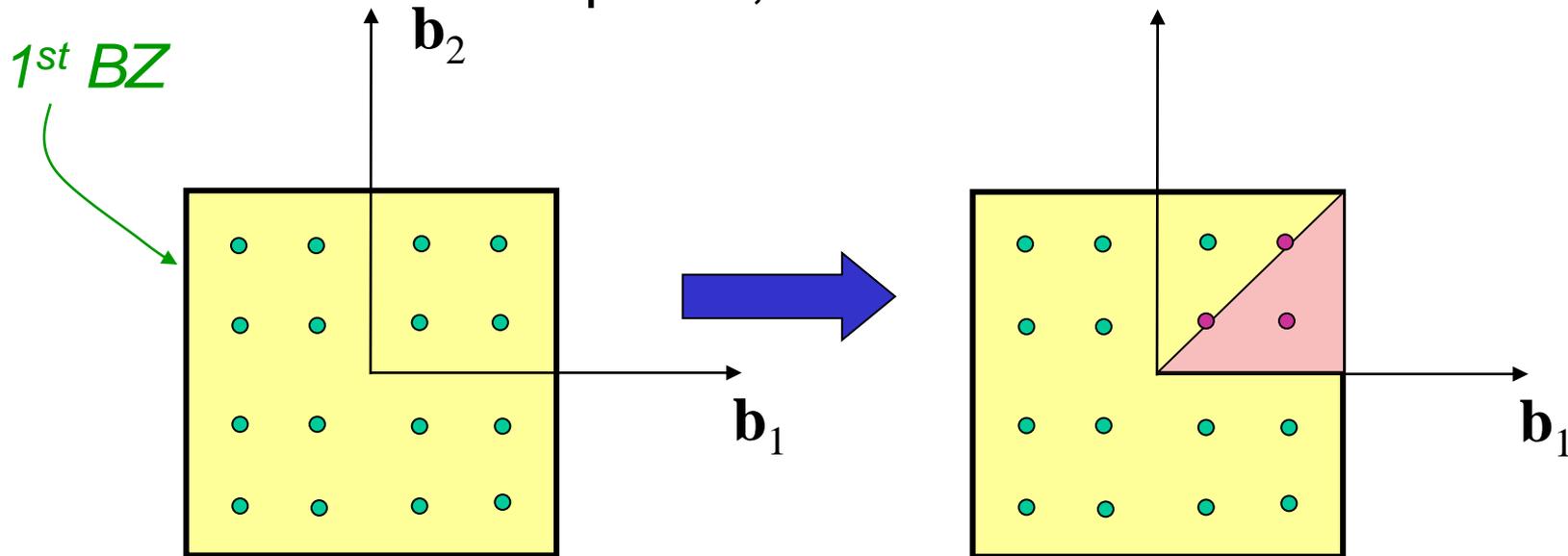
Types of k-point meshes

- **Special Points:** [Chadi & Cohen]
Points designed to give quick convergence for particular crystal structures.
- **Monkhorst-Pack:**
Equally spaced mesh in reciprocal space.
May be centred on origin [‘non-shifted’] or not [‘shifted’]



Irreducible Brillouin Zone

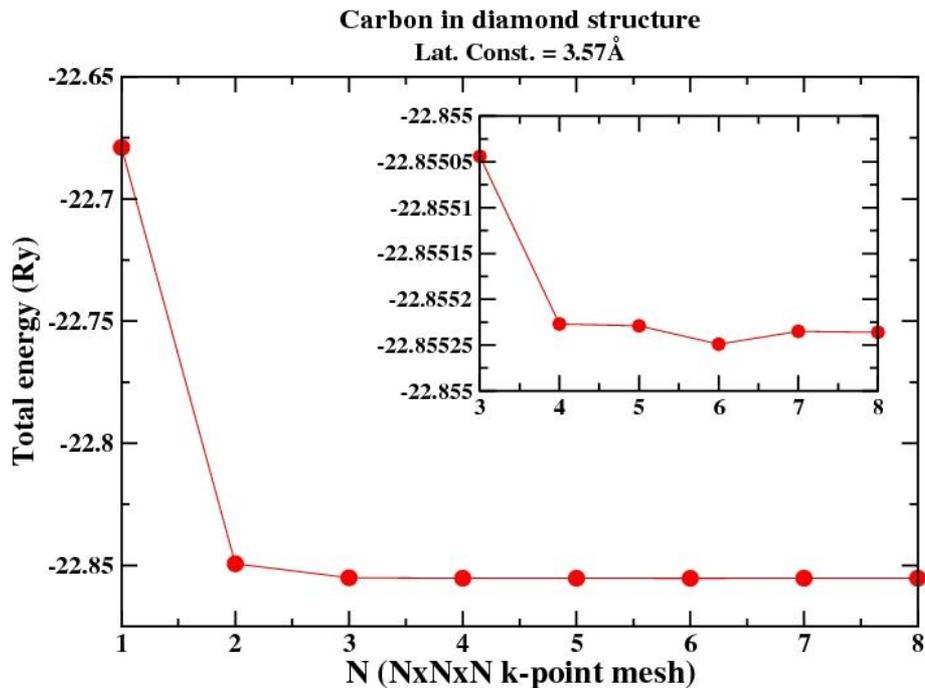
- **IBZ** depends on symmetries of system.
- Can save computational time by using appropriately weighted **k-points from IBZ** alone.
- For 'automatic' k-points, code will '**reduce**' to IBZ.



- May not want to maintain symmetries in relaxation/MD.

Input parameter `nosym`

Convergence wrt BZ sampling



Madhura Marathe

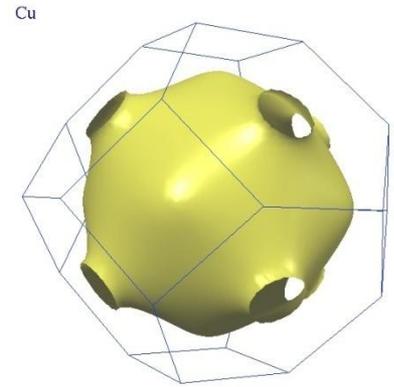
Note: Differences in energy usually converge faster than absolute value of total energy because of error cancellation (if supercells & k-points are identical or commensurate).

Problems with Metals

- Recall:

$$\langle P \rangle = \frac{\Omega}{(2\pi)^3} \sum_{n \text{ occ}} \int_{BZ} P_n(\mathbf{k}) d^3k$$

- For metals, at $T=0$, this corresponds to (for highest band) an integral over all **wave-vectors contained within the Fermi surface**, i.e., for highest band, **sharp discontinuity** in k-space between occupied and unoccupied states...need many k-points to reproduce this accurately.
- Also can lead to **scf convergence problems** because of band-crossings above/below Fermi level.
- Solve by “smearing”.



Fermi Surface of Cu
iramis.cea.fr

Smearing in Quantum-ESPRESSO

`occupations 'smearing'`

Instruction: use smearing

`smearing 'gaussian'`
`'methfessel-paxton'`
`'marzari-vanderbilt'`
`'fermi-dirac'`

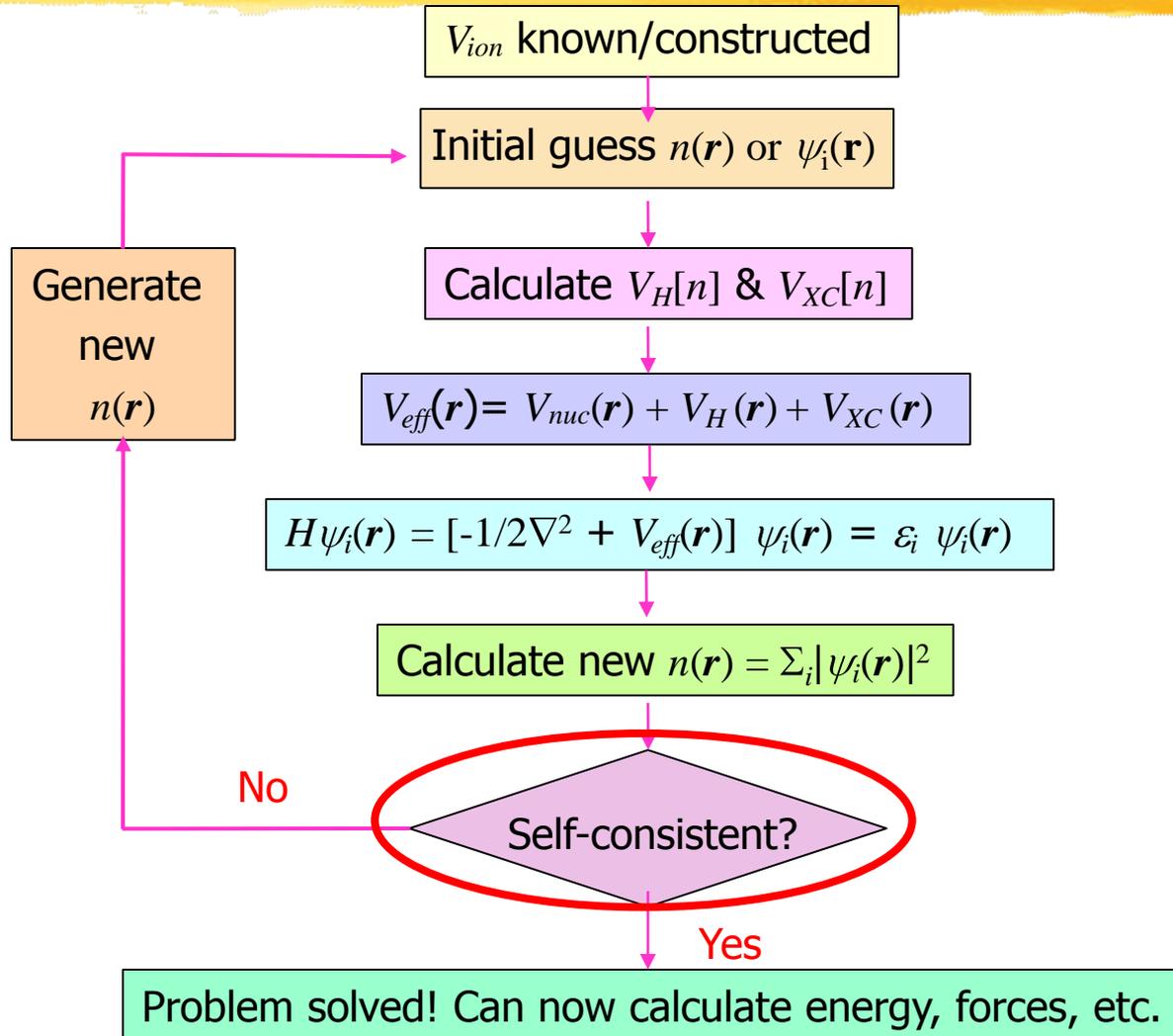
Type of
smearing

`degauss`

Smearing width

Methfessel & Paxton, Phys. Rev. B 40, 3616 (1989).
Marzari & Vanderbilt, Phys Rev. Lett. 82, 3296 (1999).

Step 7: Check if Convergence Achieved



Testing for scf convergence

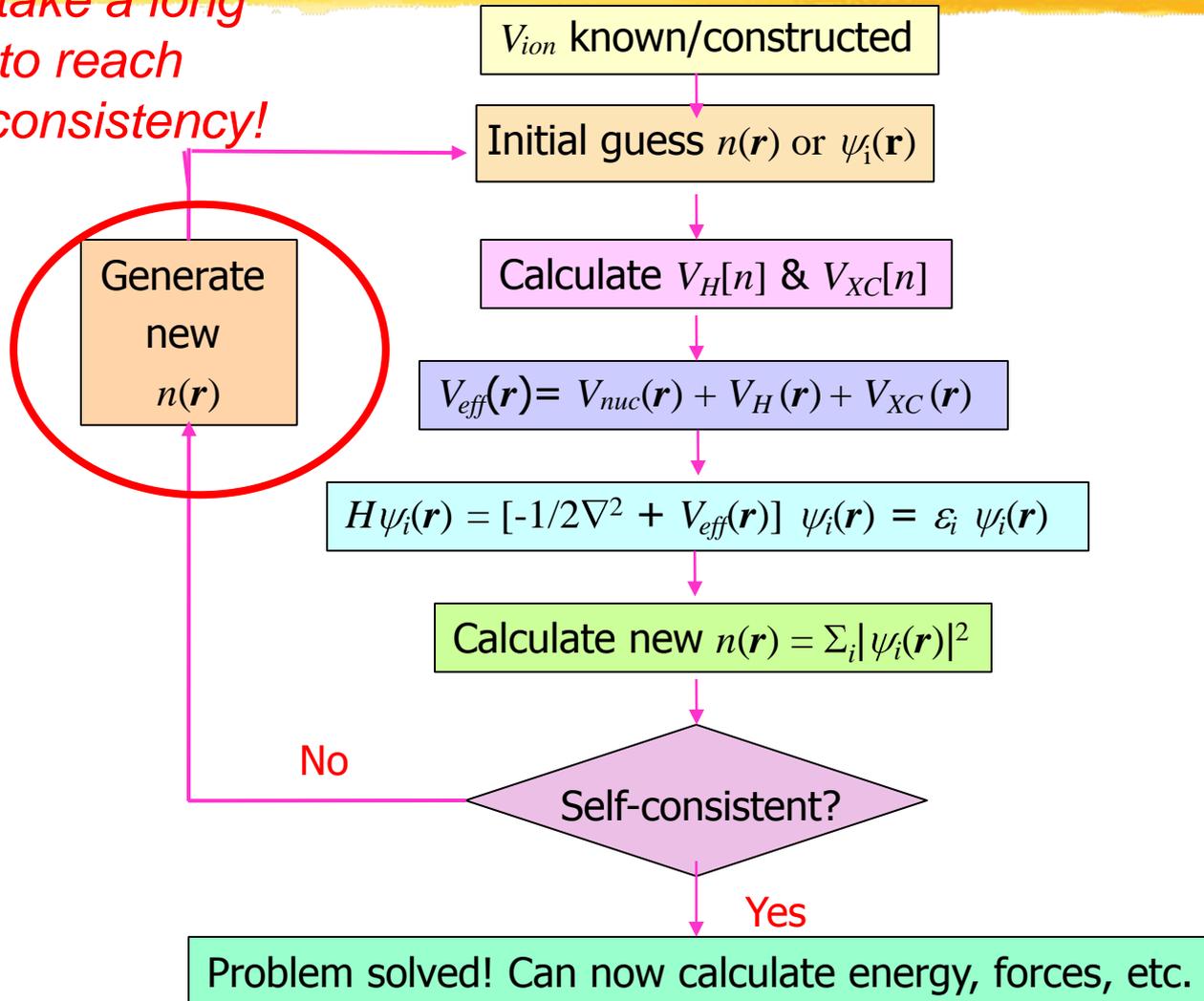
- Compare n th and $(n-1)$ th approximations for density, and see if they are close enough that self-consistency has been achieved.
- Examine squared norm of difference between the charge density in two successive iterations...should be close to zero.



Input parameter **conv_thr**

Step 8: Mixing

Can take a long time to reach self-consistency!



Mixing

- Iterations n of self-consistent cycle:
- Successive approximations to density:
 $n_{in}(n) \rightarrow n_{out}(n) \rightarrow n_{in}(n+1)$.
- $n_{out}(n)$ fed directly as $n_{in}(n+1)$?? No, usually doesn't converge.
- Need to **mix**, take some combination of input and output densities (may include information from several previous iterations).
- Goal is to achieve **self consistency** ($n_{out} = n_{in}$) in as few iterations as possible.

Mixing in Quantum-ESPRESSO



Input parameter **mixing_mode**

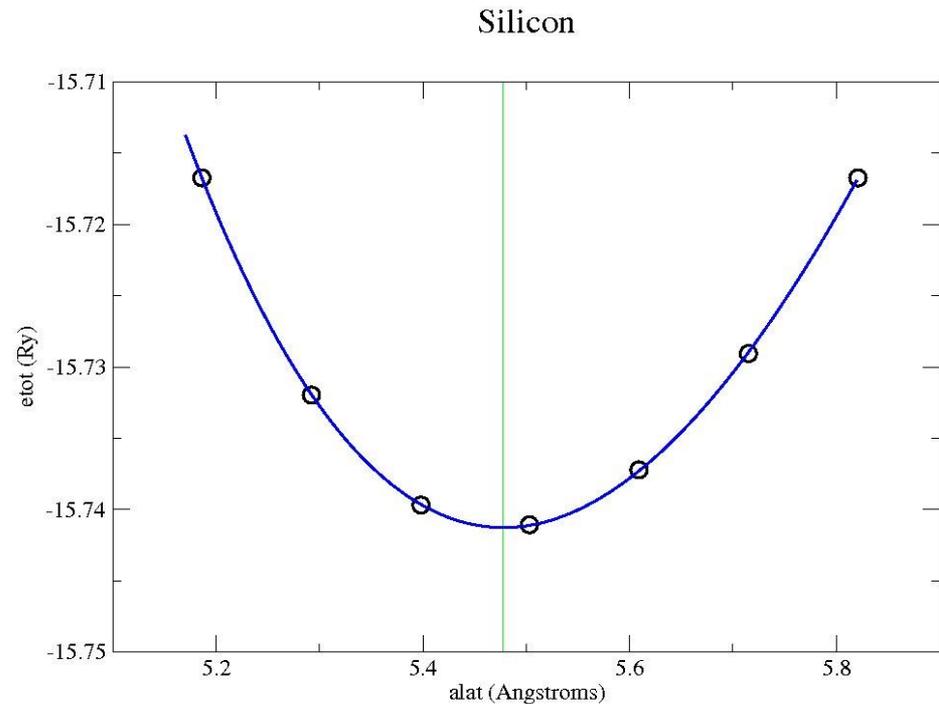
-Prescription used for mixing.

Input parameter **mixing_beta**

- How much of new density is used at each step*
- Typically use value between 0.1 & 0.7*

Output Quantities: Total Energy

- Perhaps the most important output quantity is the **TOTAL ENERGY**
- Can use, e.g., to optimize structure
- e.g., for a cubic crystal, where the structure can be specified by a single parameter (side of cube):





III. Forces & Geometry Optimization

Forces

- Need for **geometry optimization** and **molecular dynamics**.
- Could get as **finite differences** of total energy - too expensive!
- Use **force (Hellmann-Feynman) theorem**:
 - Want to calculate the force on ion I :

$$\mathbf{F}_I = -\frac{d}{d\mathbf{R}_I} \langle \Psi | H | \Psi \rangle$$

- Get three terms:

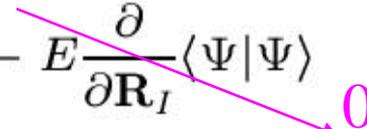
$$\mathbf{F}_I = -\langle \Psi | \frac{\partial H}{\partial \mathbf{R}_I} | \Psi \rangle - \langle \frac{\partial \Psi}{\partial \mathbf{R}_I} | H | \Psi \rangle - \langle \Psi | H | \frac{\partial \Psi}{\partial \mathbf{R}_I} \rangle$$

When $|\Psi\rangle$ is an eigenstate, $H|\Psi\rangle = E|\Psi\rangle$

-Substitute this...

Forces (contd.)

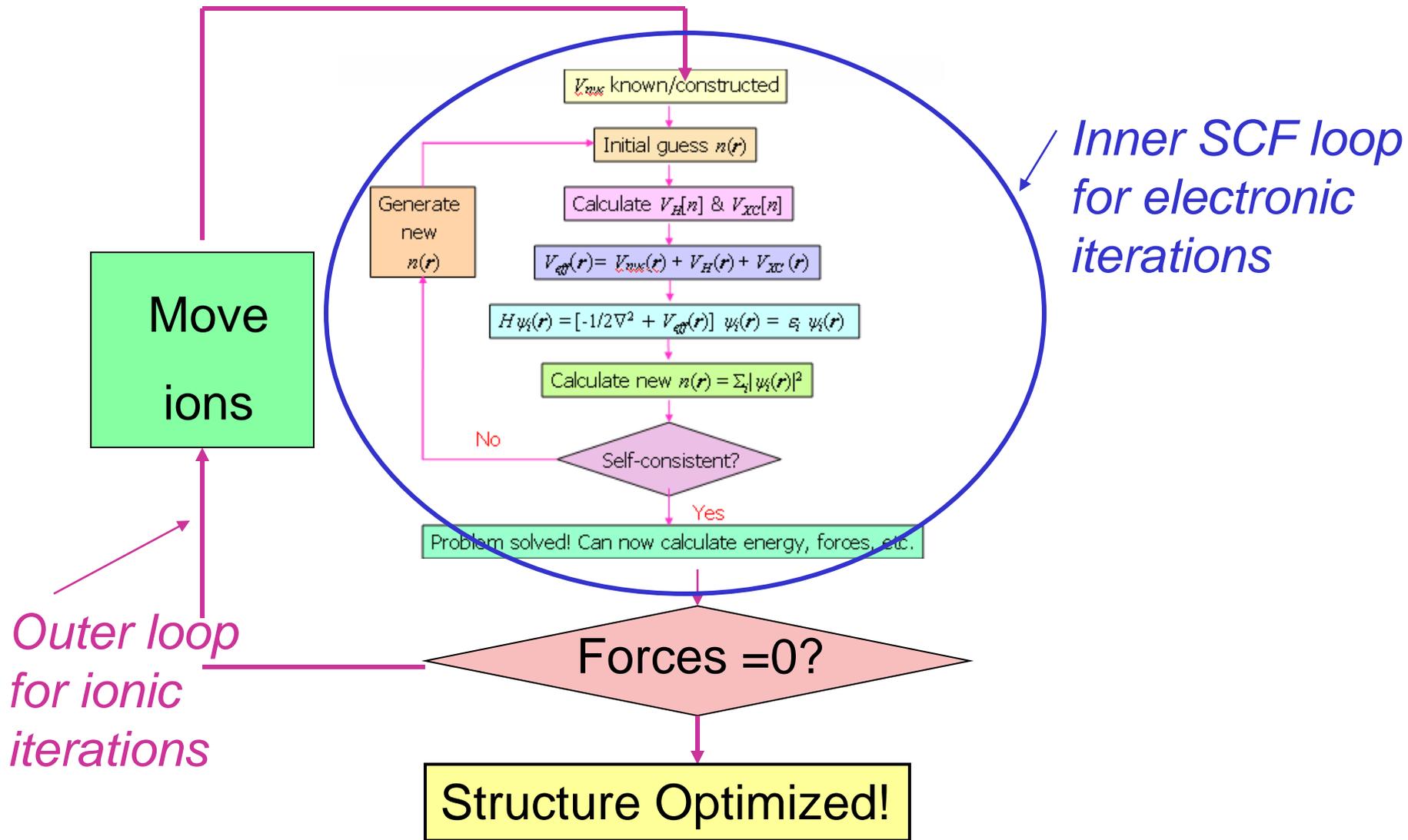
- The **force** is now given by

$$\begin{aligned}\mathbf{F}_I &= -\langle \Psi | \frac{\partial H}{\partial \mathbf{R}_I} | \Psi \rangle - E \langle \frac{\partial \Psi}{\partial \mathbf{R}_I} | \Psi \rangle - E \langle \Psi | \frac{\partial \Psi}{\partial \mathbf{R}_I} \rangle \\ &= -\langle \Psi | \frac{\partial H}{\partial \mathbf{R}_I} | \Psi \rangle - E \frac{\partial}{\partial \mathbf{R}_I} \langle \Psi | \Psi \rangle\end{aligned}$$


- Note that we can now **calculate the force** from a calculation at **ONE configuration alone** – huge savings in time.
- If the basis depends upon ionic positions (not true for plane waves), would have extra terms = **Pulay forces**.
- $|\Psi\rangle$ should be exact eigenstate, i.e., scf well-converged!

Input parameter `tprnfor`

An Outer Loop: Ionic Relaxation



Geometry Optimization With Forces

- Especially useful for optimizing internal degrees of freedom, surface relaxation, etc.

```
calculation = 'relax'
```

- Choice of algorithms for ionic relaxation, e.g., steepest descent, BFGS.

```
NAMELIST &IONS
```

```
Input parameter ion_dynamics
```



IV. Structure of PWscf Input Files

PWscf input file

- For documentation about input parameters for PWscf, read **INPUT_PW.html** in the **Doc** subdirectory.
- The PWscf input file is structured into **NAMELISTS** and **INPUT_CARDS**.

PWscf NAMELISTS in Input File

- There are three mandatory **NAMELISTS** :
- **&CONTROL** input variables that control the type of calculation performed and the amount of I/O.
- **&SYSTEM** input variables that specify the system.
- **&ELECTRONS** input variables that control the algorithms used to reach a self-consistent solution of the Kohn-Sham equations.
- There are other (optional) namelists...

PWscf INPUT_CARDS in Input File

- There are three mandatory **INPUT_CARDS**:
- **ATOMIC_SPECIES** name, mass and pseudopotential used for each species in system.
- **ATOMIC_POSITIONS** coordinates of each atom in unit cell.
- **K_POINTS** coordinates and weights of the k-points used for BZ sums..
- There are other (optional) INPUT_CARDS...

Other Features / Types of Calculations

- Spin Polarized Calculations (Magnetism)
- Density Functional Perturbation Theory (Phonons)
- Nudged Elastic Band (Barriers)
- Molecular Dynamics
- ...and much, much more!



*It's not a **bird**...*

*It's not **Superman**...*

*It's a **Plane Wave** !*

The End!

Have fun with Quantum-ESPRESSO!

