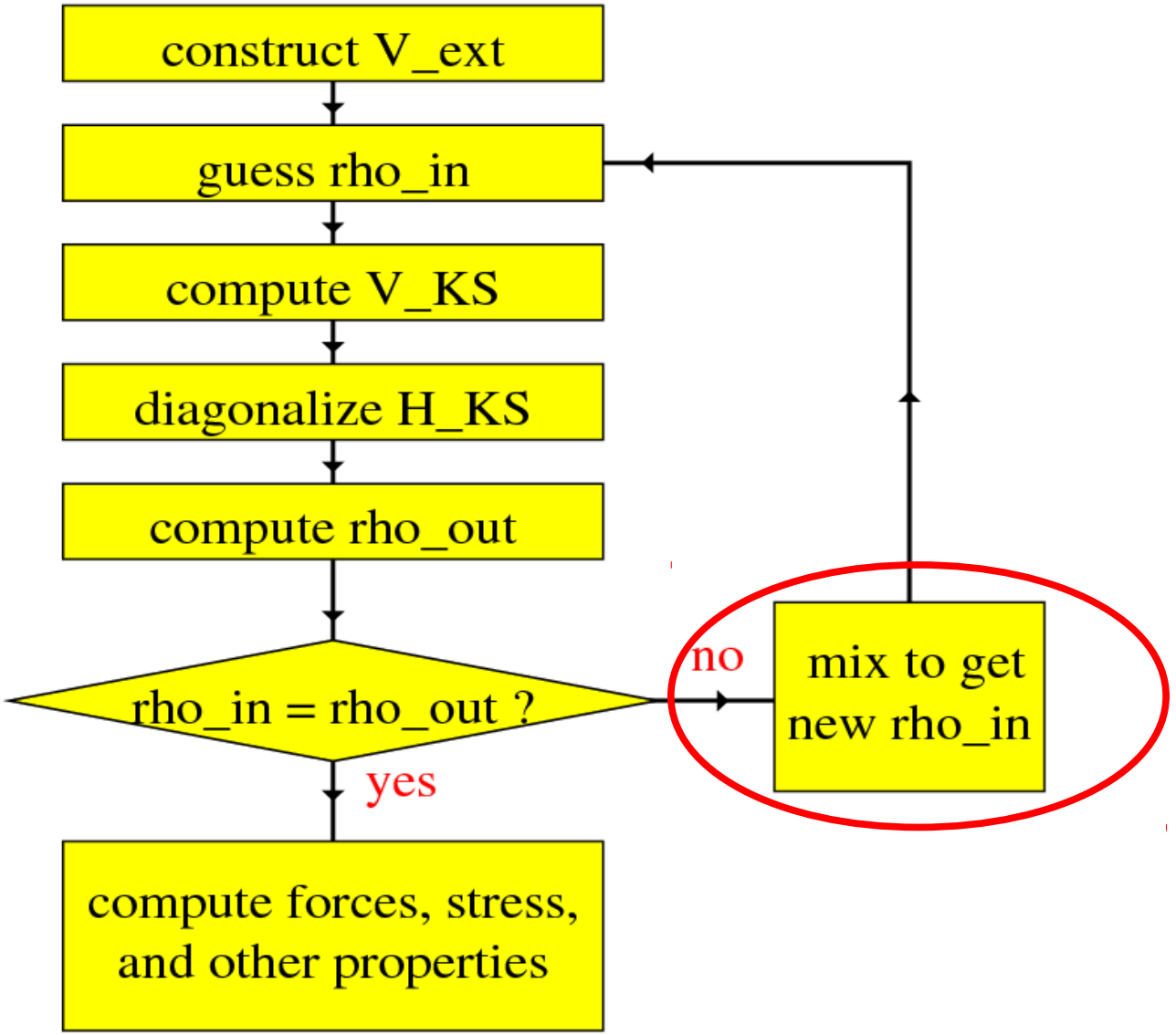
Step 7 : mixing



Mixing

Once iteration n of the self-consistent cycle has completed … how to get next guess for rho ?

direct iteration in which rho_out is fed directly in rho_in

$$\text{rho\_in}(n) \rightarrow \text{rho\_out}_t(n) \rightarrow \text{rho\_in}(n+1)$$

usually doesn't converge.

One needs to mix, take some combination of input and output densities (may include information from several previous iterations).

Goal is to achieve self consistency (rho_out=rho_in) in as few iterations as possible.

Mixing

Simplest prescription: linear mixing

rho_in(n+1) = beta * rho_out(n) + (1-beta) rho_in(n).

Usually slow but should converge for small enough values of beta

There exist more sophisticated prescriptions (Broyden mixing, modified Broyden mixing of various kinds…) based on Quasi Newton Raphson methods.

Input parameter mixing_mode

plain | *TF*| *local-TF*

Input parameter mixing_beta

-Typical values between 0.1 & 0.7

(depend on type of system)

Broyden Mixing

$$\rho^i_{in} = \overline{\rho} + \delta\rho^i_{in} \longrightarrow \rho^i_{out} = \overline{\rho} + \delta\rho^i_{out}$$

In the linear regime if M iterations have been accumulated

$$\rho_{in} = \rho^M_{in} + \sum_{i=1}^{M-1} \alpha_i(\rho^i_{in} - \rho^{i+1}_{in}) \longrightarrow \rho_{out} = \rho^M_{out} + \sum_{i=1}^{M-1} \alpha_i(\rho^i_{out} - \rho^{i+1}_{out})$$

BM determines ρ^{best}_{in} and ρ^{best}_{out} in the already explored manifold by minimizing the norm of $\Delta\rho_{I/O}$ w.r.t. the α_i coefficients and then applies SM to them.

$$\rho^{new}_{in} = \rho^{best}_{in} + \beta\Delta\rho^{best}_{I/O} = (1-\beta)\rho^{best}_{in} + \beta\rho^{best}_{out}$$

Simple Mixing Revisited

Ideally one would like

$$\rho_{in}^{new} = \rho_{in} - \delta\rho_{in} = \overline{\rho}$$

but we only have access to

$$\Delta\rho_{I/O} = -\chi_0\chi^{-1}\delta\rho_{in}$$

If some simple approximation A to $\chi\chi_0^{-1}$ is available one can then use it to improve the new trial density

$$\delta\rho_{in} \approx A\Delta\rho_{I/O}$$

$$\rho_{in}^{new} = \rho_{in} + \beta A\Delta\rho_{I/O} \approx \rho_{in} - \beta\delta\rho_{in}$$

Thomas-Fermi screening can provide a useful approximate inverse; for very inhomogeneous systems a local TF scheme may be required.