

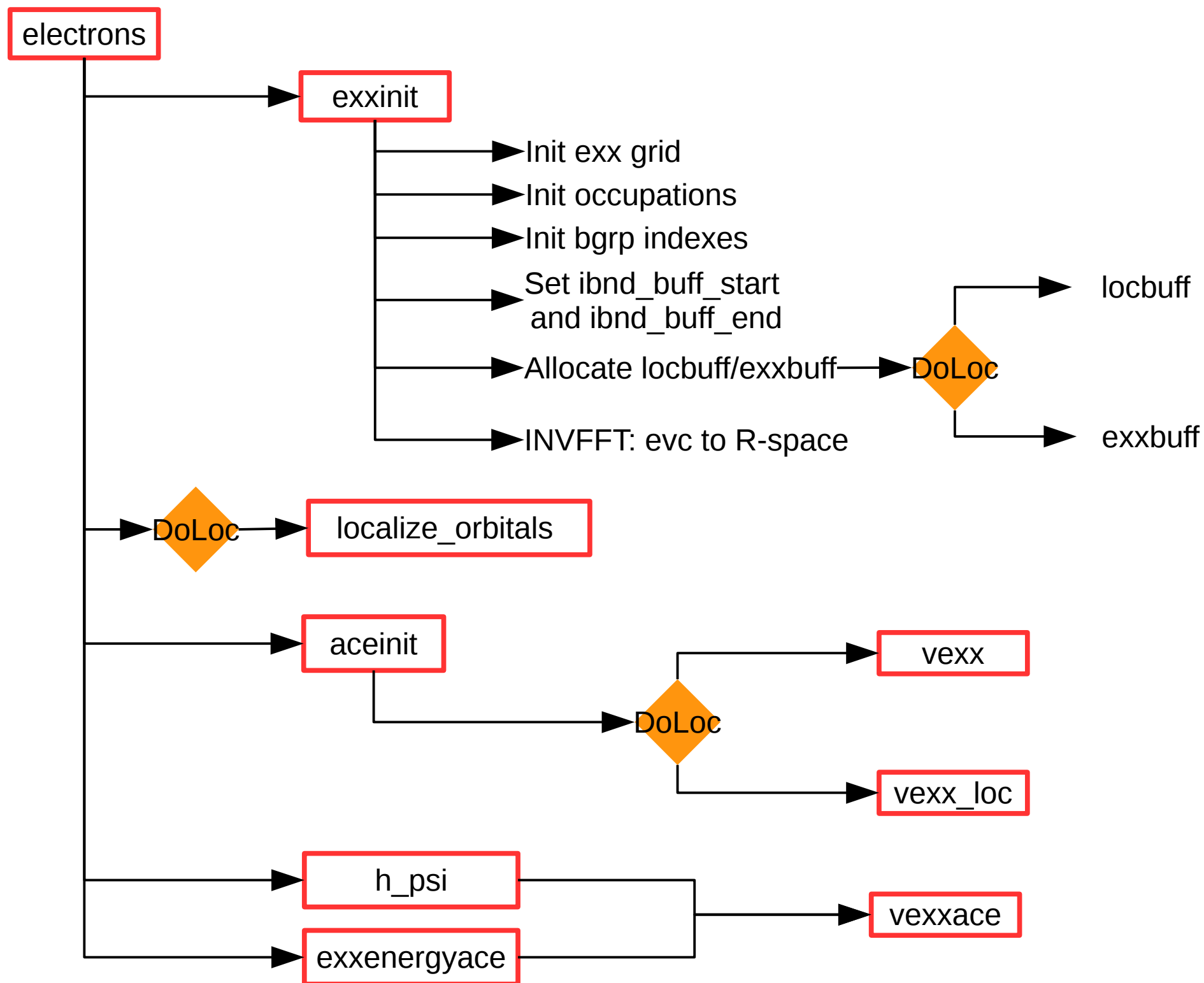
Status and perspectives in the exact exchange code in QE

SCDM localization in pw.x (loc_scdm.f90)

- Localization as a general purpose analysis tool (also for DFT), e.g. dipole moments, print/visualize localized orbitals
- How many subroutines for dipole moment calculations?
 - Modules/compute_dipole.f90
 - PW/src/compute_dip.f90
- SCDM-k for exact exchange with K-points

Exact exchange code in pw.x (exx.f90)

- Extending L-ACE to K-points (and USPP?)
- Reduced boxes: Poisson solver or small FFTs
- Some smart parallelization can be combined with L-ACE
- Code reorganization:
 - Memory management
 - Still retain NO-ACE or remove it?



Exact exchange code in pw.x

exxinit

separate initialization from invfft

wfc G to/from R space is used many times in the code. Could we do a general purpose driver which does it for arbitrary grids? Is it worth?

real buffer for ALL gamma_only calculations (currently only with DoLoc=.true.). exxinit should not know about localization

vexx

decide what to do with the old NO-ACE method

fork between L-ACE and BP-ACE: memory

use some low memory routine by default and use the high memory routine only when necessary (BG)

Memory deployment

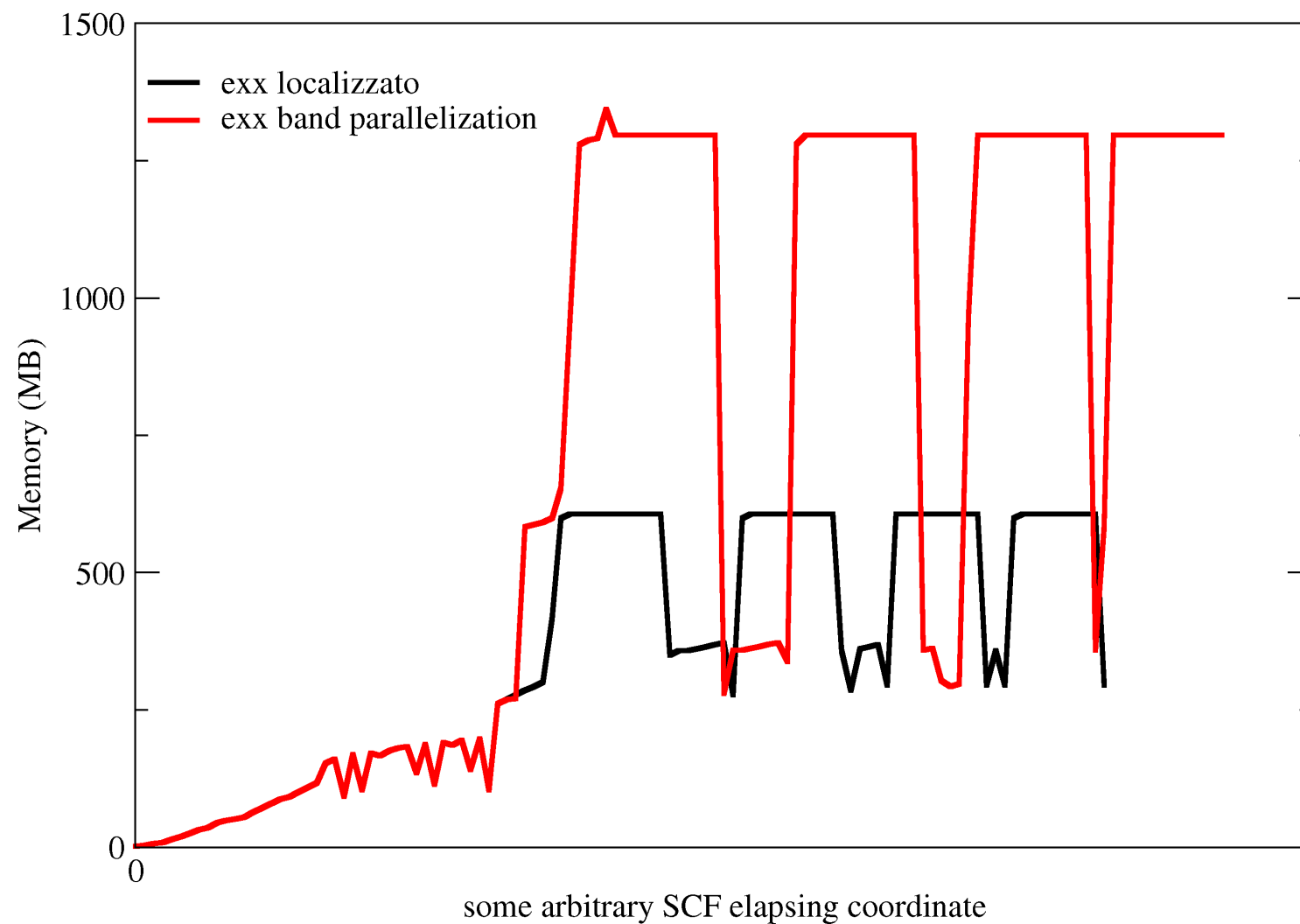
When trying to go towards large system the main bottleneck is a memory crash.

The CPU times are reasonable:

237 water molecules, 80 Ry took from 25 to 2 hours using L-ACE with different thresholds

(with 576 cores and 118 GB)

Memory deployment



Memory deployment

L-ACE (vexx_loc)

fac	48485	(NPW)
rhoc	216000	(NGrid)
vc	216000	(NGrid)
result	216000 X 8	(NGrid X Nbnd)

**Non-scaling
allocations**

ACE (vexx_gamma)

temppsic_dble	216000	(NGrid)	CODE NO ACE
temppsic_aimag	216000	(NGrid)	CODE NO ACE
psiwork	216000	(NGrid)	CODE NO ACE
result_g	6027	(NGrid)	
exxtemp	216000 X 1 X 7	(NGrid X NPol X Nbnd)	
rhoc	216000 X 8	(NGrid X Nbnd)	
vc	216000 X 8	(NGrid X Nbnd)	
result	216000 X 8	(NGrid X JBlock)	