SCF Preconditioners within Abinit

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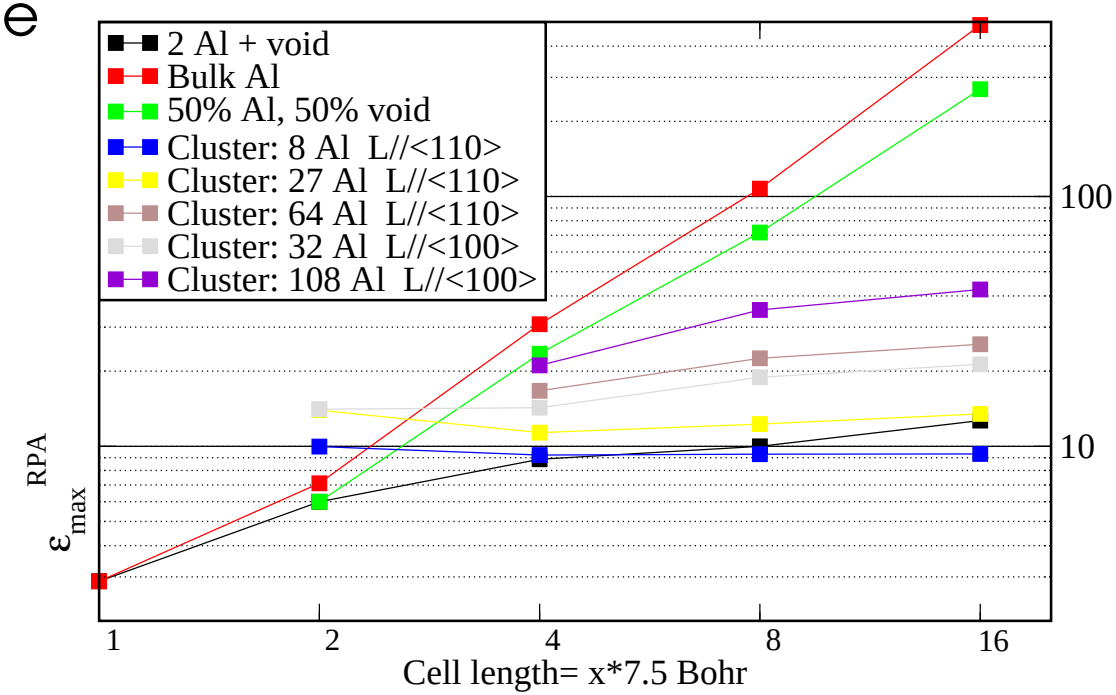
Plan

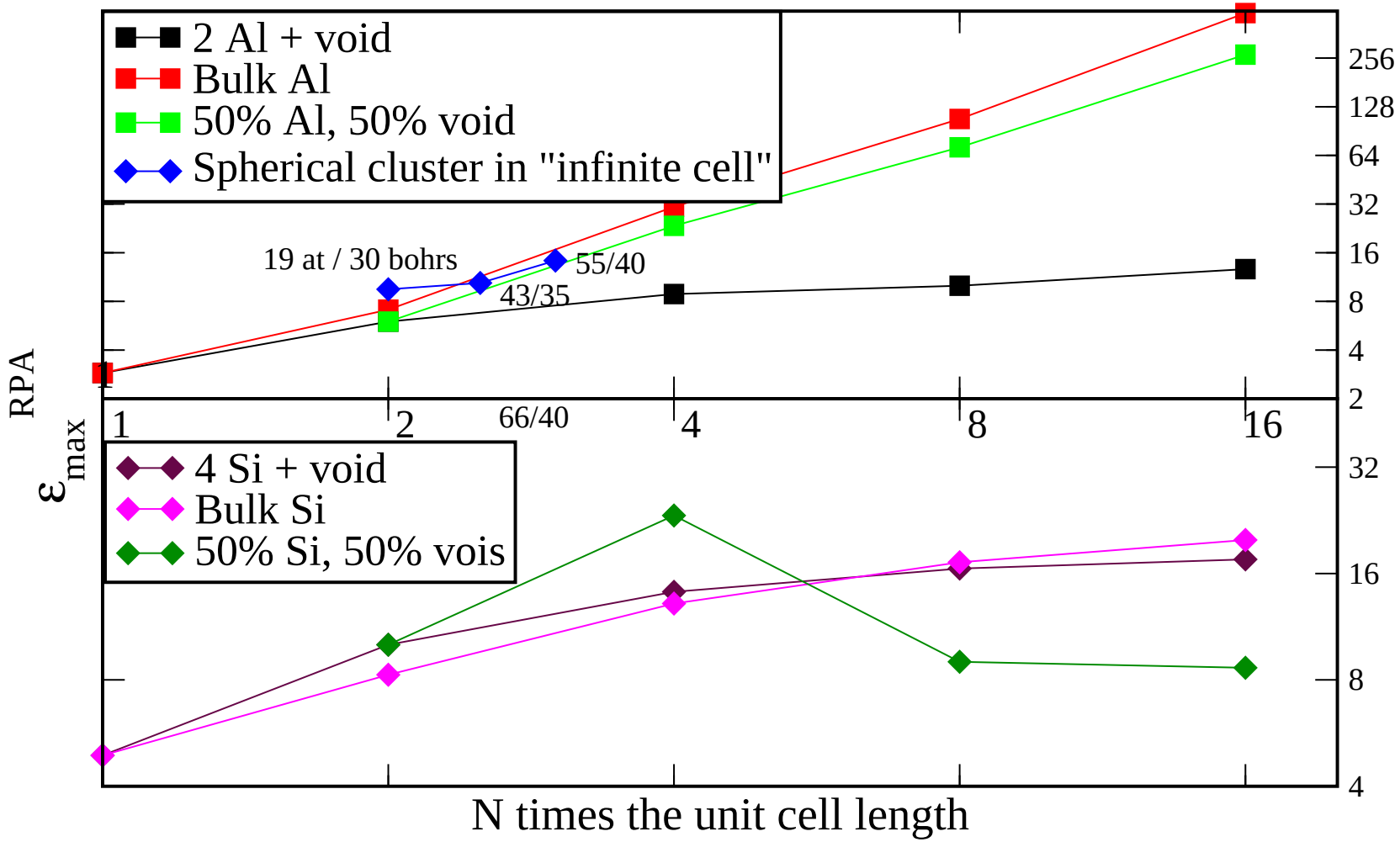
- Reminder: Why would one uses preconditioners?
  - Convergence problems
  - History coping algorithms and preconditioners
- From Ho's Newton-Raphson Method to *extrapolar*
  - Newton-Raphson on SCF cycles
  - The extrapolar approximation
- From Kerkers's preconditioner to *RSKerker*
  - Kerkers's preconditioner for metals
  - Abinit's extended Kerker's scheme
  - RSKerker
- Conclusion

Reminder: Convergence problems

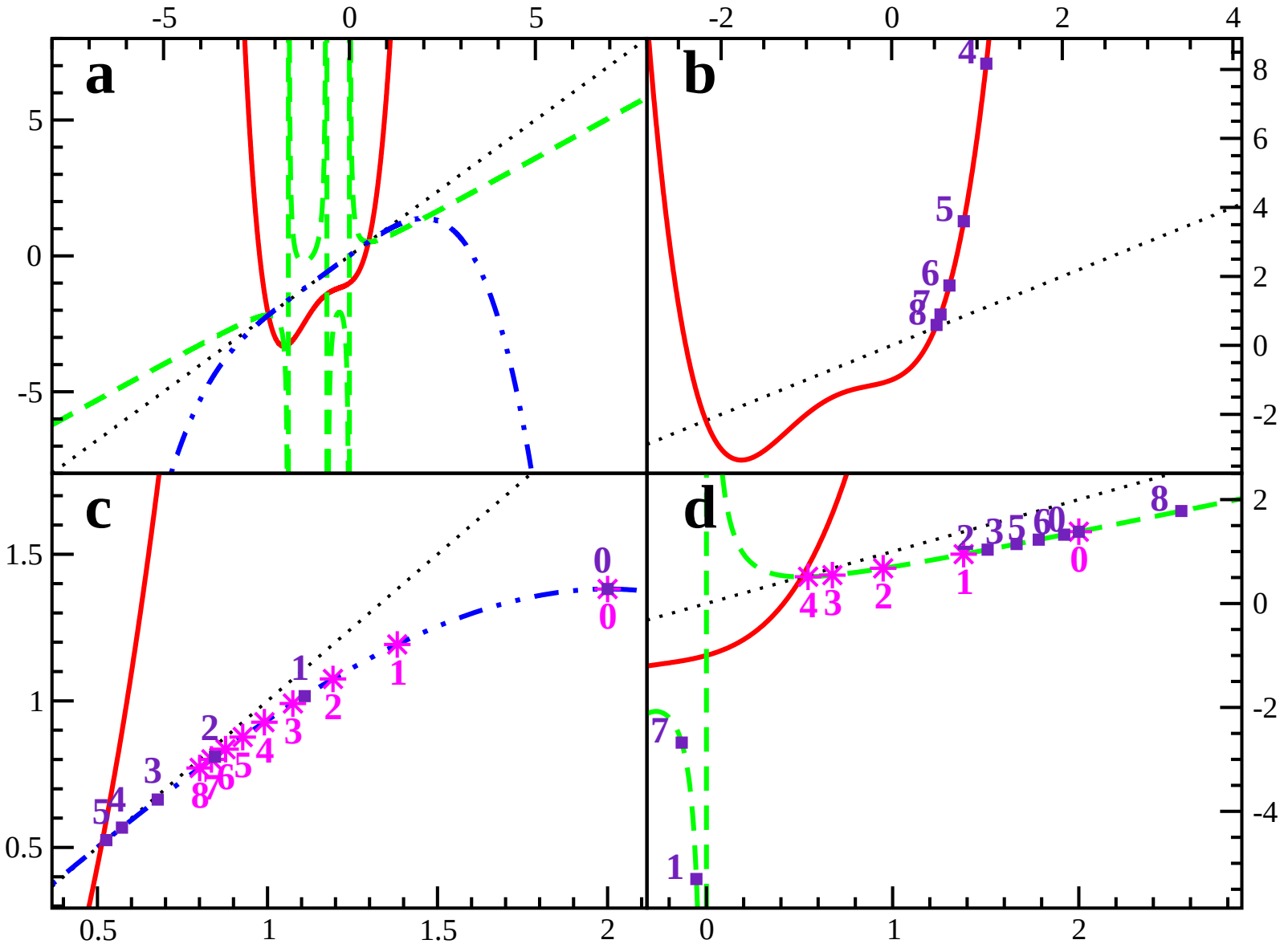
- Charges react to error in the trial potential ($\propto r^2$).
- The matrix of coefficient discribing this reaction (the hessian) is called the dielectric permittivity matrix.
- Reaction can amplify the error.
- Basically the largest eigenvalue of the dielectric permittivity matrix will show the difficulty for getting convergence



Reminder: Convergence problems



Reminder: History and preconditioners



Reminder: Why would one uses preconditioners?

- Hessians of large systems have large maximum eigenvalues.
- Simple mixing is not enough because the problem complexity is a matter of condition number (CN)$= \frac{\lambda_{max}}{\lambda_{min}}$.
  - The smallest eigenvalues (λ_{min})) depends on the XC. They are more or less local properties.
  - The largest eigenvalues (λ_{max})) basically grows with system size.
- Advanced mixing schemes use a single mixing coefficient per step which is not enough to cope with difficult problem.
- To evaluate the efficiency of a preconditioner we must stick with simple mixing.

Exact Newton-Raphson's preconditioning 1/2

- K.-M. Ho *et. al.*, PRB 25, no. 6, p. 4260 (1982)
-

$$\chi(G,G') = -2\sum_{n,n',k}(w_{n,k}-w_{n,k'})\frac{\langle nk|e^{-iG.r}|n'k\rangle\langle nk|e^{iG.r}|n'k\rangle}{E_{n',k}-E_{n,k}}$$

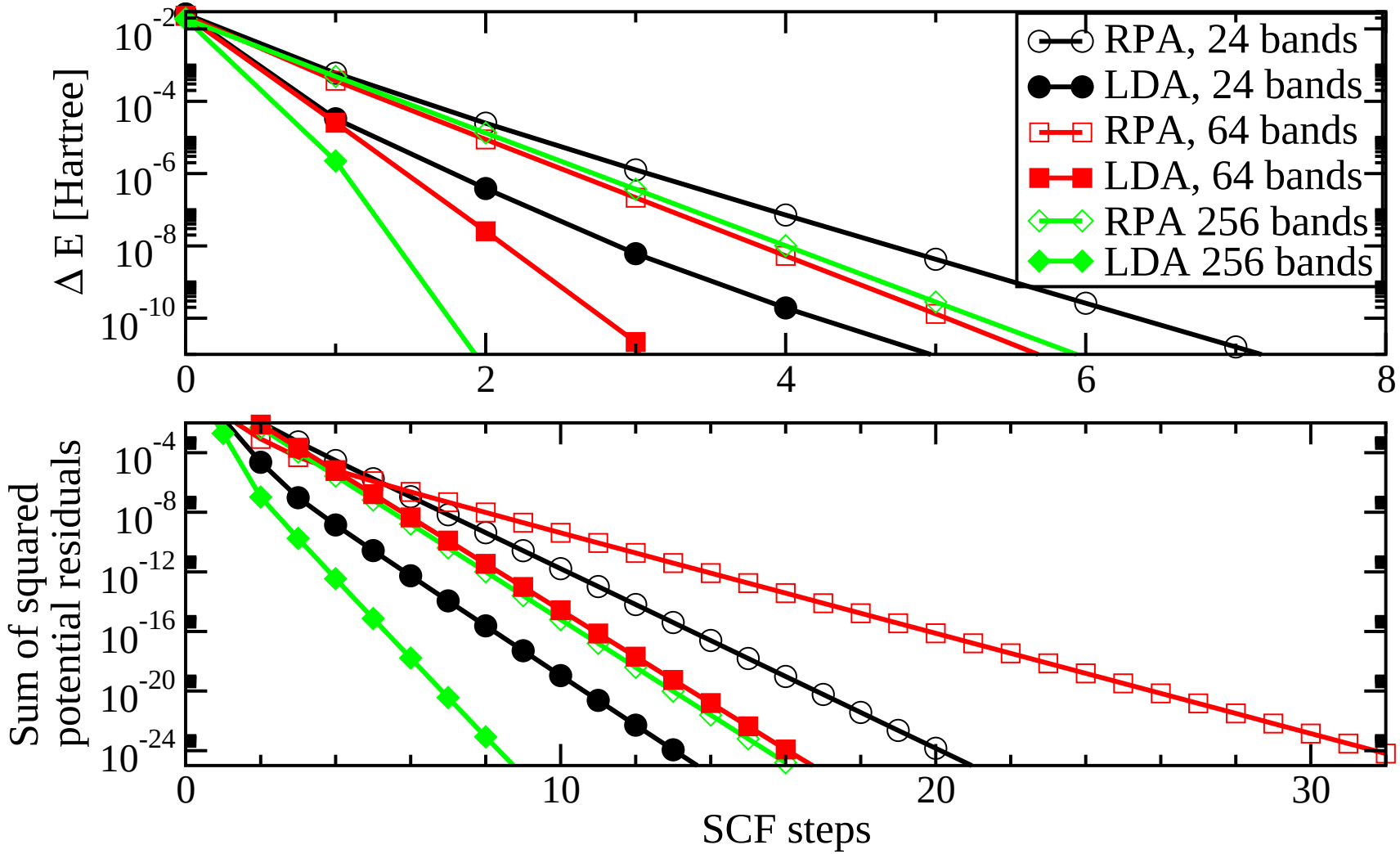
$$\varepsilon_{LDA}(G,G') = \delta_{G,G'} - \frac{4\pi e^2}{\Omega_c G^2}\chi(G,G')$$

$$+ \frac{\beta e^2}{3}\left(\frac{3}{\pi}\right)^{\frac{1}{3}}\sum_{G''}\rho^{\frac{-2}{3}}(G-G'')\chi(G'',G')$$

$$\varepsilon_{RPA}(G,G') = \delta_{G,G'} - \frac{4\pi e^2}{\Omega_c G^2}\chi(G,G')$$

Exact Newton-Raphson's preconditioning 2/2

- Linear cell of bulk Si (8 atoms) with no longitudinal symmetry.



Extrapolar 1/3

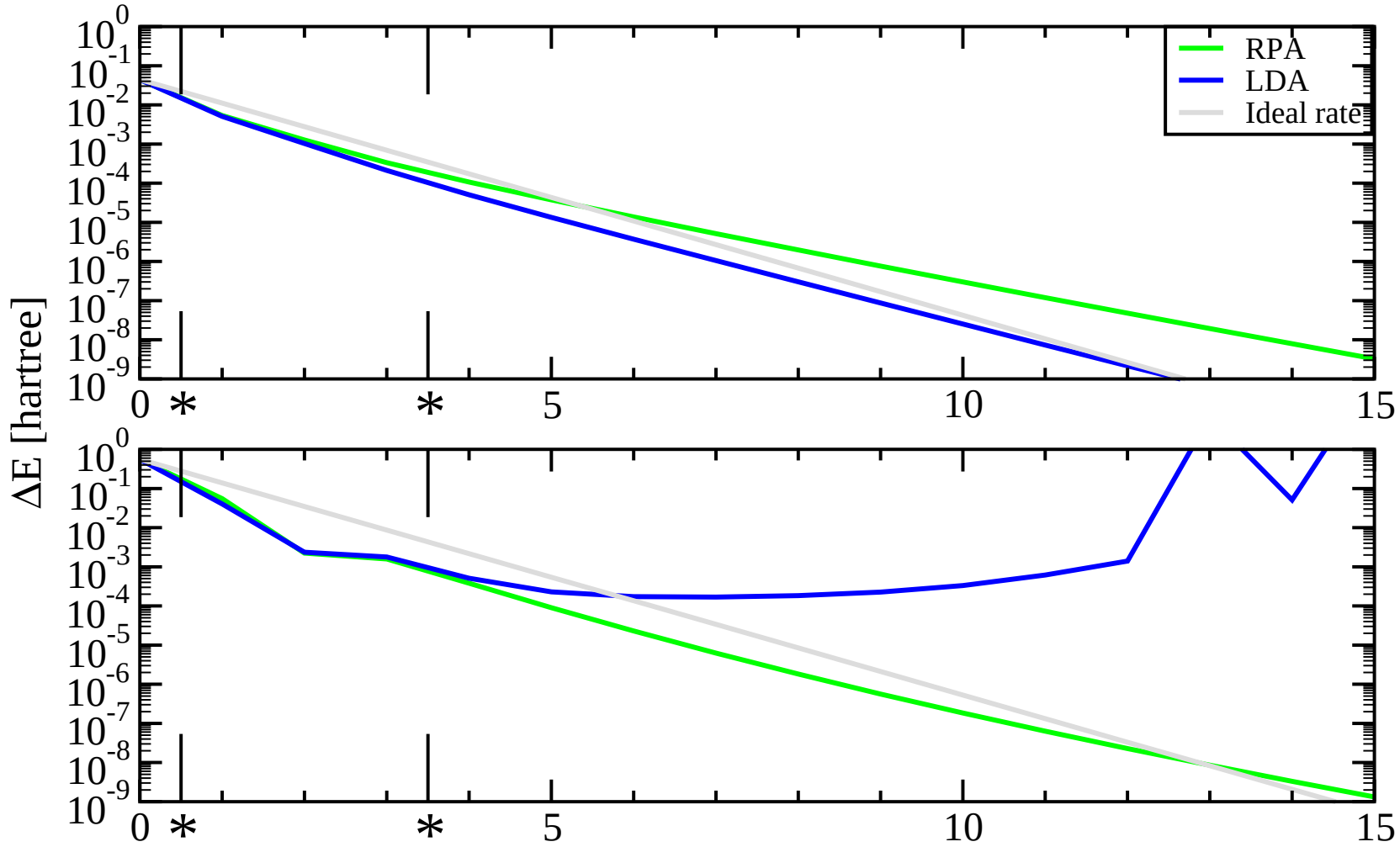
- Best known to Abinit users as iprcel $\neq 0$.
- $$\chi_k(G,G') \propto A_k + \alpha \sum_{n=1}^{n_{valence}} \sum_{n'=n_{band}+1}^{\infty} \frac{\psi^*_{kn}(r)\psi_{kn'}(r)\psi^*_{kn'}(r)\psi_{kn}(r')}{\bar{E}-E_{kn}}$$

$$\chi_k(G,G') \propto A_k + \alpha \sum_{n=1}^{n_{valence}} \frac{\psi^*_{kn}(r)\psi_{kn}(r)}{\bar{E}-E_{kn}} - \alpha \sum_{n=1}^{n_{valence}} \sum_{n'=1}^{n_{band}} \frac{\psi^*_{kn}(r)\psi_{kn'}(r)\psi^*_{kn'}(r)\psi_{kn}(r')}{\bar{E}-E_{kn}}$$

- Two (extra) parameters $\alpha = dielam$ et $\bar{E} = diegap$.

Extrapolar 2/3

- Linear cell of bulk (resp. slab) Si, 16 (resp. 8) atoms, with no longitudinal symmetry.



Extrapolar 3/3

- Advantages of extrapolar:
  - A (very) reduced plane wave basis can be used to compute the polarizability matrix (0.5 Ha may be enough !);
  - Extrapolar is much faster to apply than Ho's method;
  - Almost useless to tune parameters.
- drawbacks:
  - Must be used within RPA for inhomogeneous systems;
  - Do not converge as efficiently as Ho's method;
  - Still an $O(N^4)$ method (scaling figures later).

Kerker's preconditioner

- G.P. Kerker, PRB, vol. 23, nb. 6, p. 3082 (1981)
- Rewrite Poisson's equations:

$$(\nabla^2 - \lambda^2)V_{coul} = -4\pi\left(\rho + \frac{\lambda^2}{4\pi}V_{coul}\right)$$

- Apply this to an SCF cycle (in reciprocal space) :

$$V_{coul}^{(n+1)} = \frac{4\pi\rho^{(n)} + \lambda^2 V_{coul}^{(n)}}{4\pi^2 G^2 + \lambda^2}$$

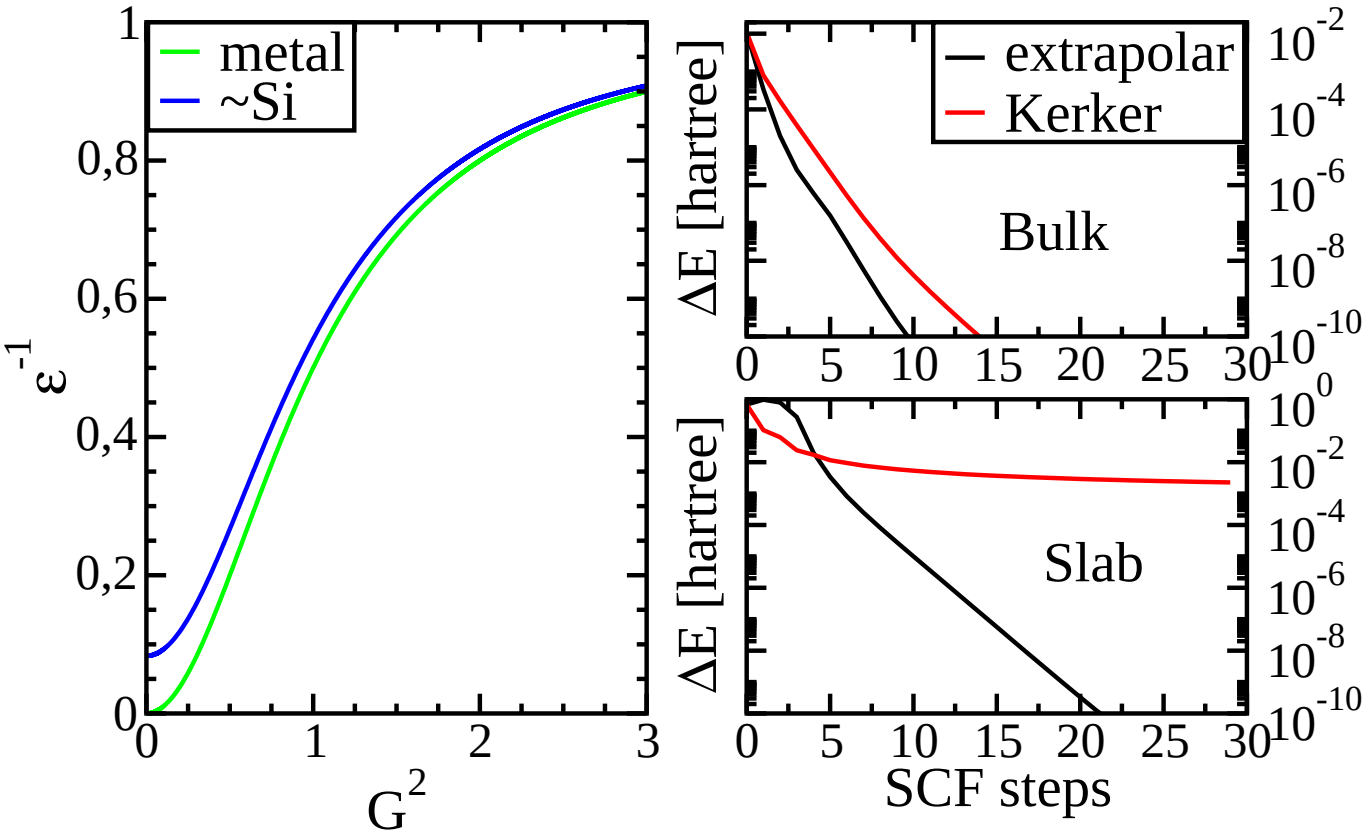
- We get (changing $\lambda \rightarrow \Lambda = \frac{2\pi}{\lambda} =$ dielng):

$$V_{coul,res}^{prc} = \frac{\Lambda^2 G^2}{\Lambda^2 G^2 + 1} V_{coul,res}$$

Abinit's extended Kerker's scheme

- Can be applied on the full trial potential.
- Can be tuned to account for finit charge sloshing (diemac= ε_r):

$$V_{res}^{prc} = \frac{\frac{1}{\varepsilon_r} + \Lambda^2 G^2}{\Lambda^2 G^2 + 1} V_{res}$$



RSKerker

- Kerker is equivalent in real space to:

$$\left(1-\frac{\Lambda^2}{4\pi^2}\nabla^2\right)V_{prc}(\boldsymbol{r})=\left(\frac{1}{\varepsilon_r}-\frac{\Lambda^2}{4\pi^2}\nabla^2\right)V_{res}(\boldsymbol{r})$$

- V_{prc} is minimizing:

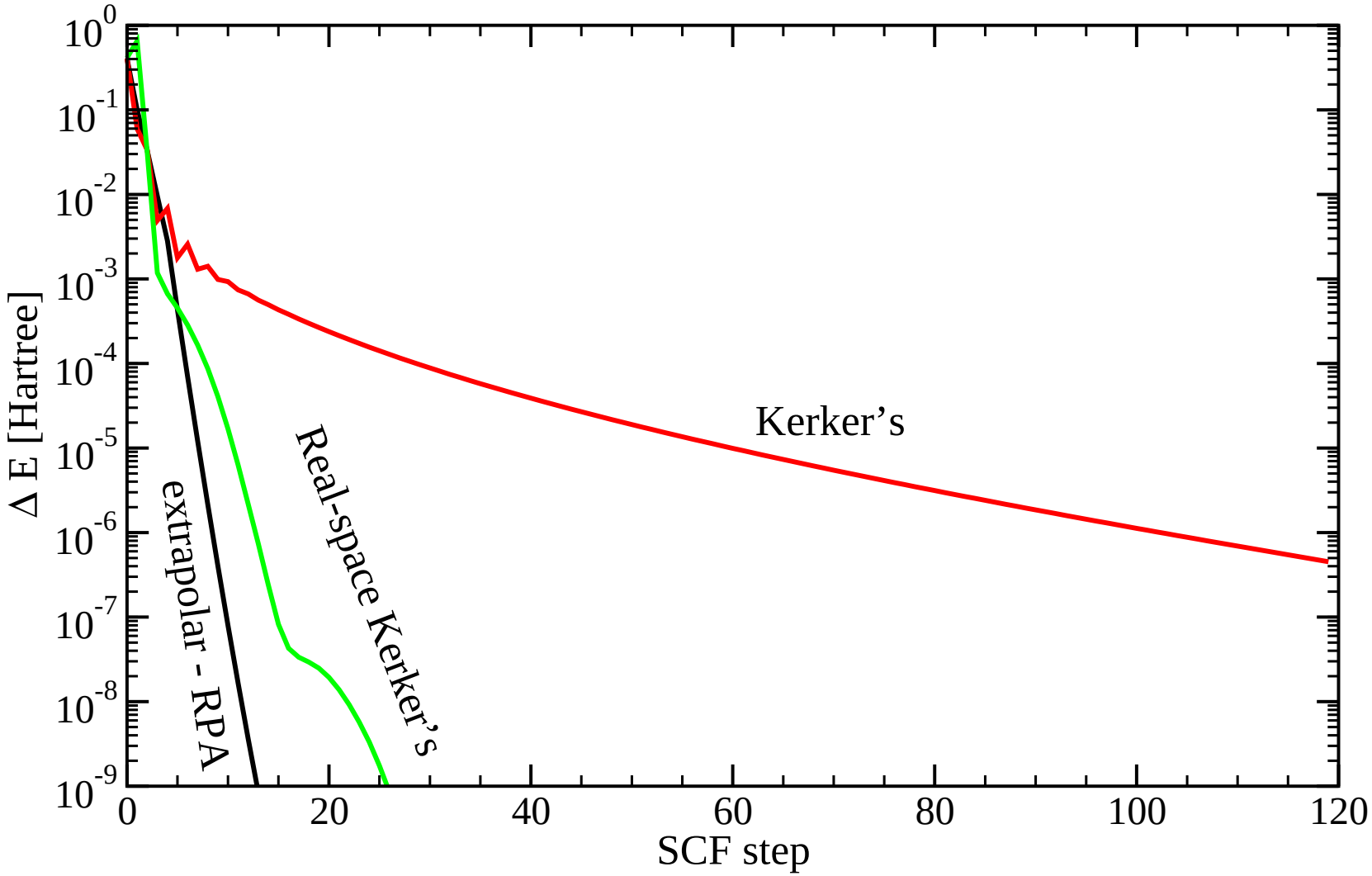
$$\text{pf}\,(V)=\frac{1}{2}V.\left(1-\frac{\Lambda^2}{4\pi^2}\nabla^2\right)V-V.\left(\frac{1}{\varepsilon_r}-\frac{\Lambda^2}{4\pi^2}\nabla^2\right)V_{res}$$

- We can change $\varepsilon_r \longrightarrow \varepsilon_r(r)$
- First intuitive choice for $\varepsilon_r(r)$ is

$$\varepsilon_r(r) \propto \rho + Cste$$

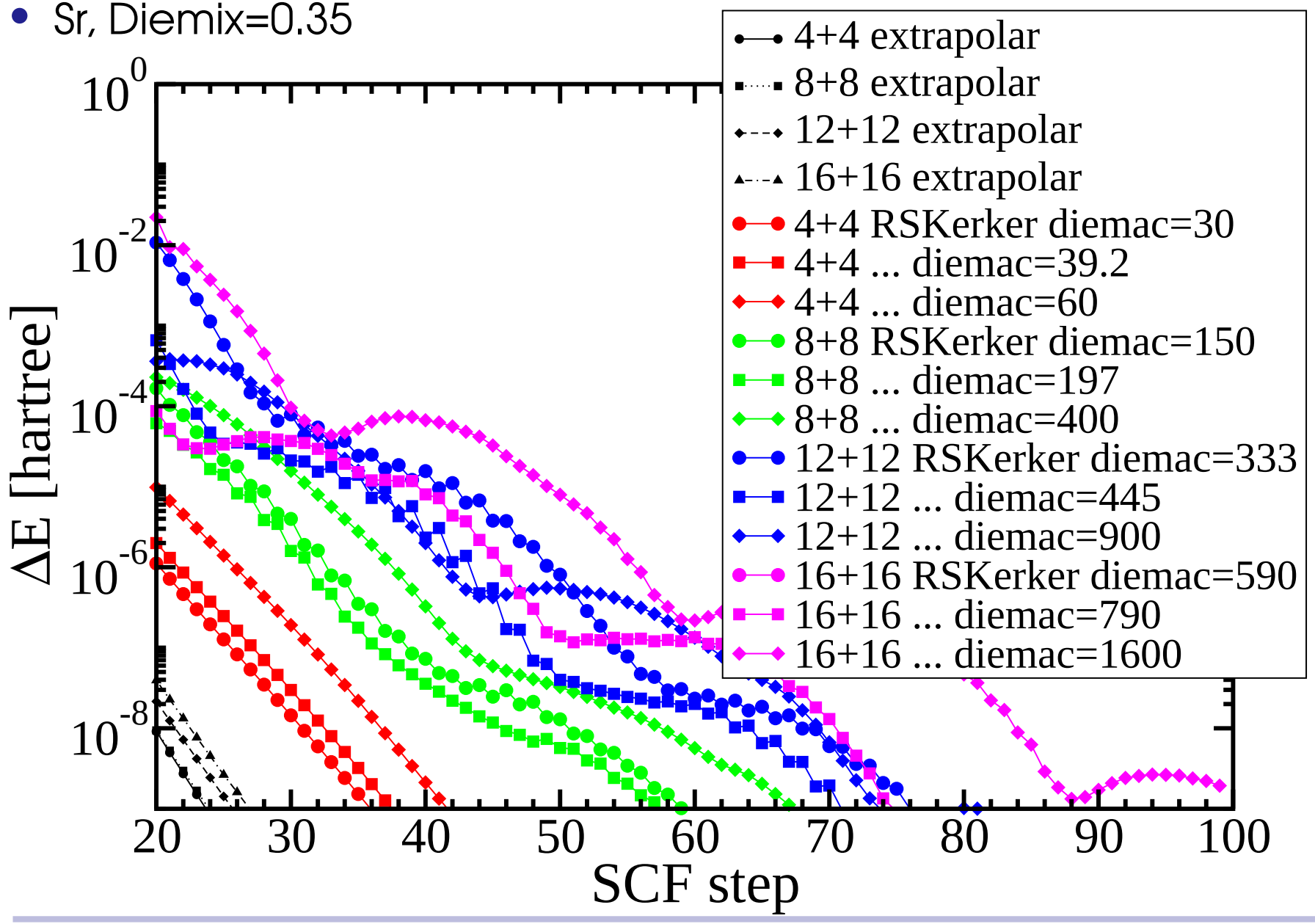
RSKerker

- Cell of 12 Al, 12 Vacuum.

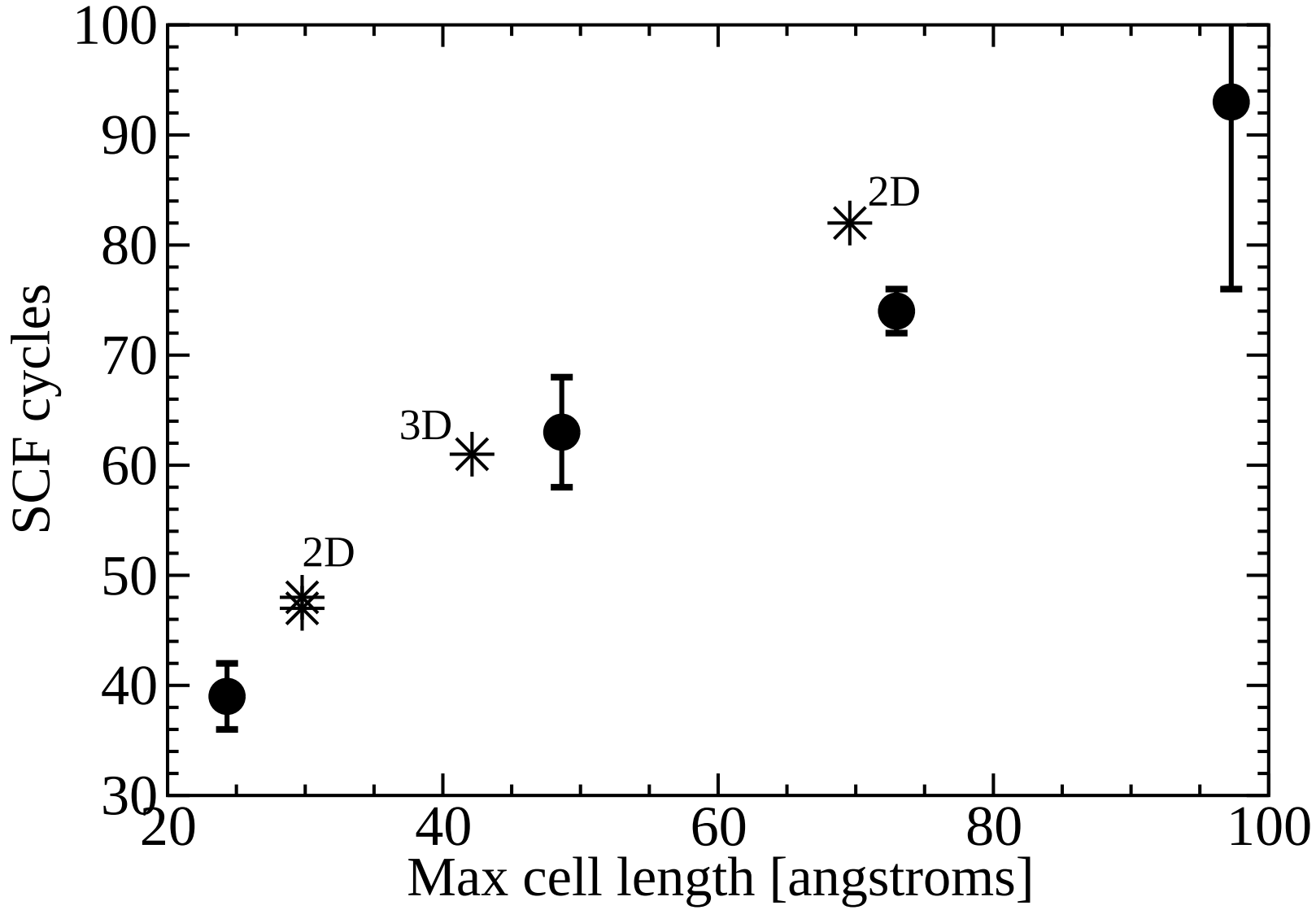


RSKerker

- Sr, Diemix=0.35

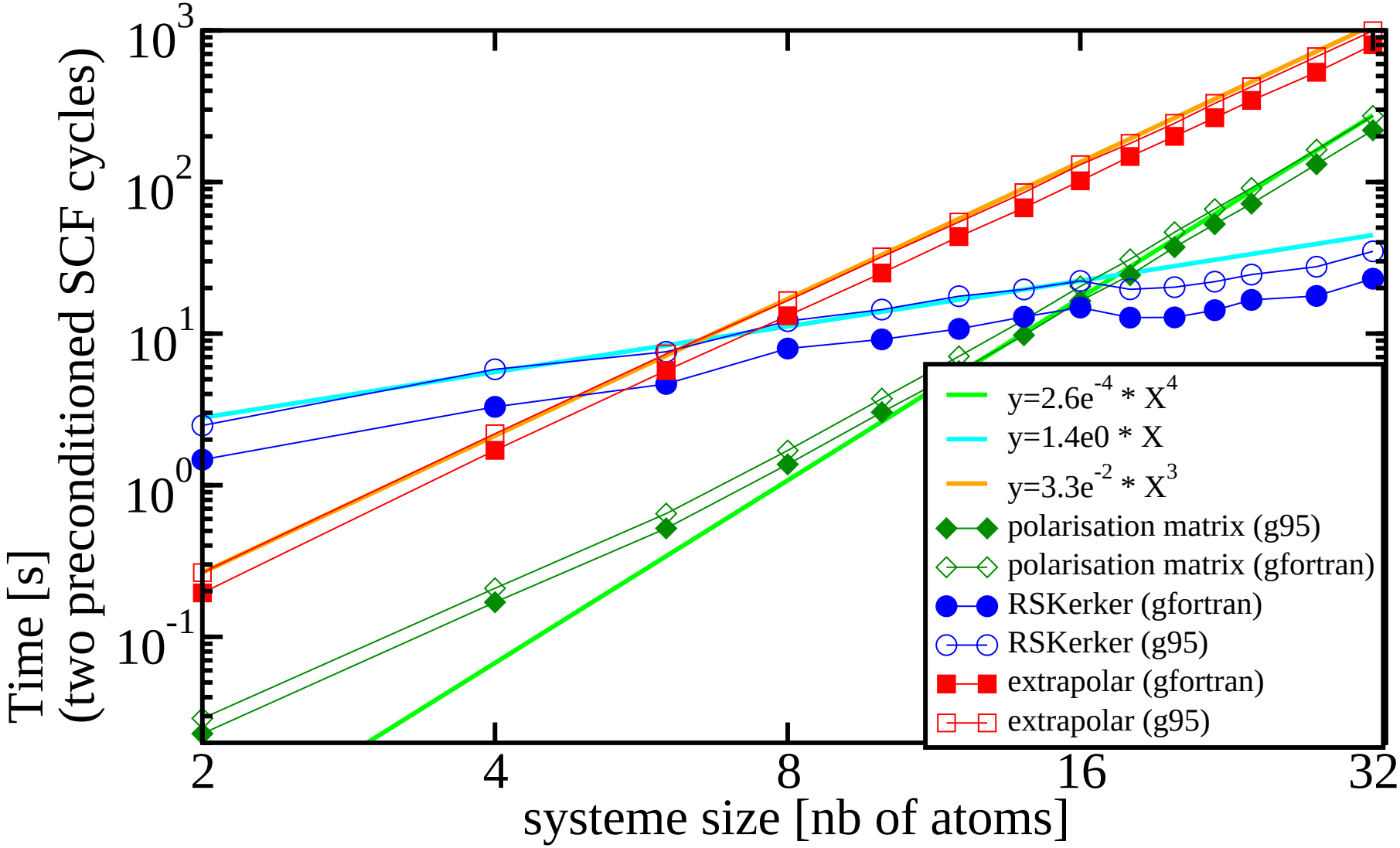


- Sr, Diemix=0.35



Scaling

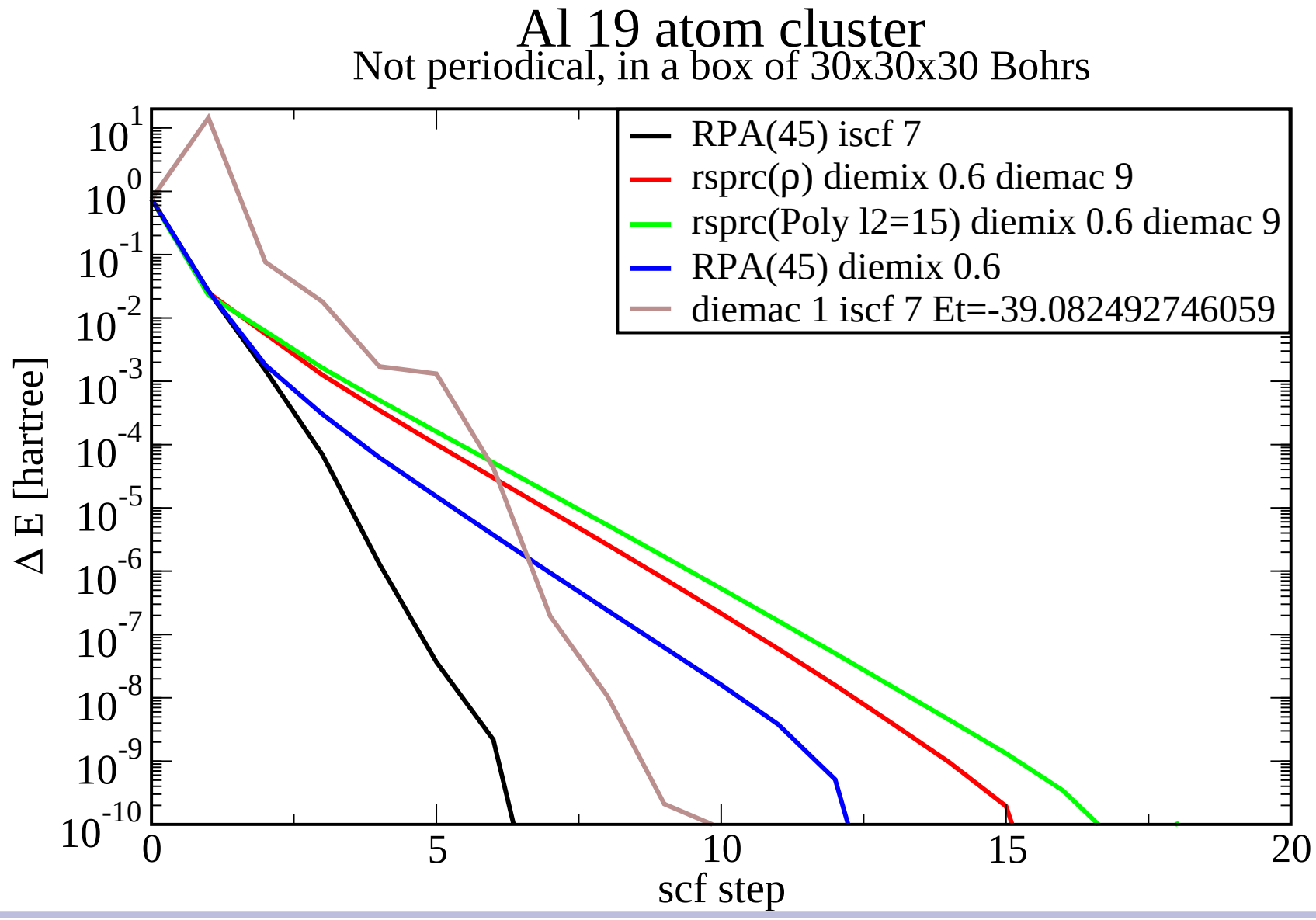
- Timings taken in Sr (diecut=2 Ha, ecut=6 Ha)



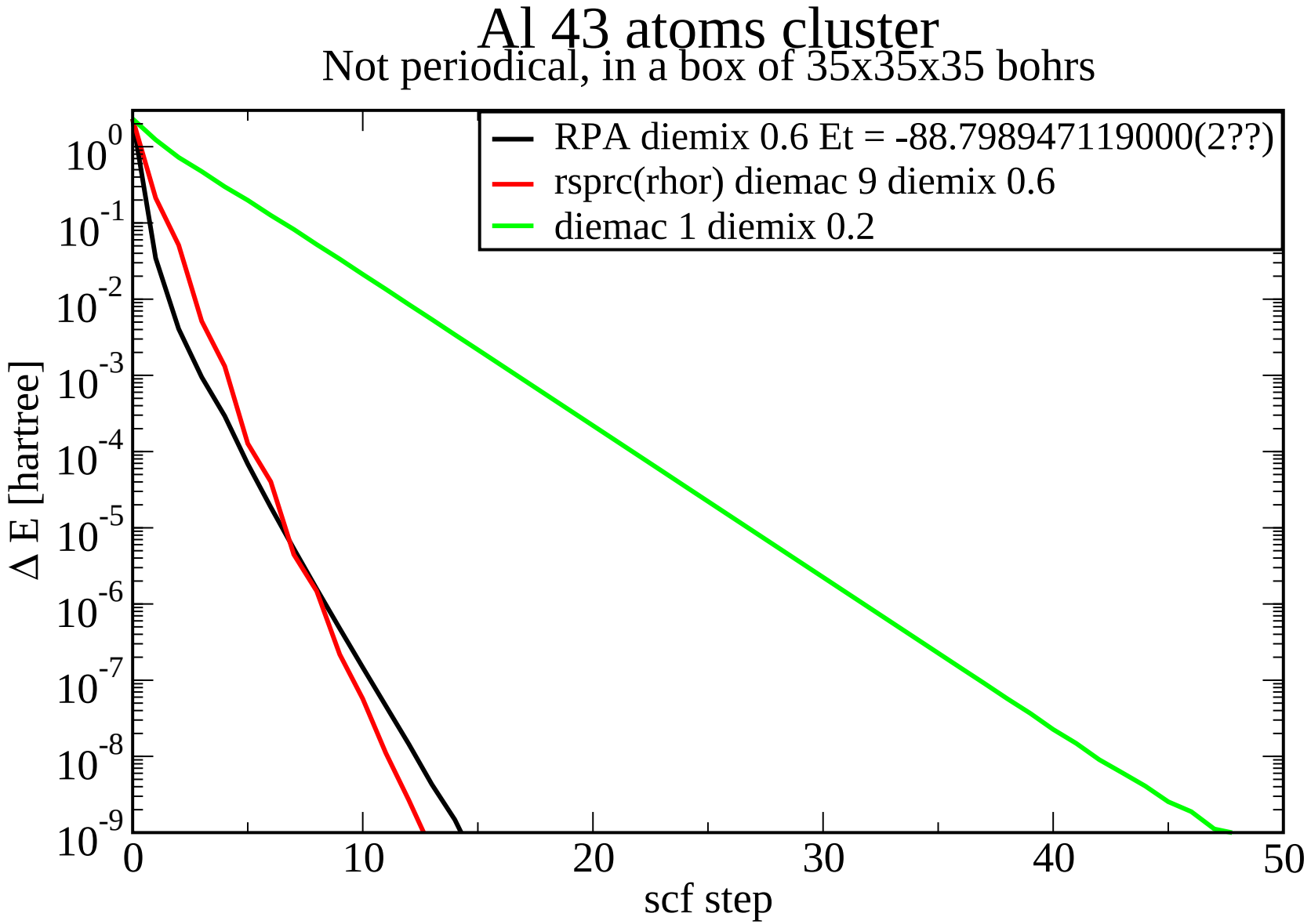
Conclusion

- Extrapolar is perfect for all medium sized systems but the scaling will prevent the use for larger systems. However trying to keep reducing the prefactor might be fruitfull.
- RSKerker is very promising for largest systems; yet it needs much better approximation for the real-space dielectric function. Uses of a $\Lambda(r)$ is also possible.

BIGDFT pcpm


Al 19 atom cluster
Not periodical, in a box of 30x30x30 Bohrs
RPA(45) iscf 7
rsprc(ρ) diemix 0.6 diemac 9
rsprc(Poly l2=15) diemix 0.6 diemac 9
RPA(45) diemix 0.6
diemac 1 iscf 7 Et=-39.082492746059
Δ E [hartree]
scf step
10^1
10^0
10^-1
10^-2
10^-3
10^-4
10^-5
10^-6
10^-7
10^-8
10^-9
10^-10
0
5
10
15
20

BIGDFT pcpm


Al 43 atoms cluster
Not periodical, in a box of 35x35x35 bohrs
RPA diemix 0.6 Et = -88.798947119000(2??)
rsprc(rhor) diemac 9 diemix 0.6
diemac 1 diemix 0.2
Δ E [hartree]
scf step
10^0
10^-1
10^-2
10^-3
10^-4
10^-5
10^-6
10^-7
10^-8
10^-9
0
10
20
30
40
50

BIGDFT pcpm

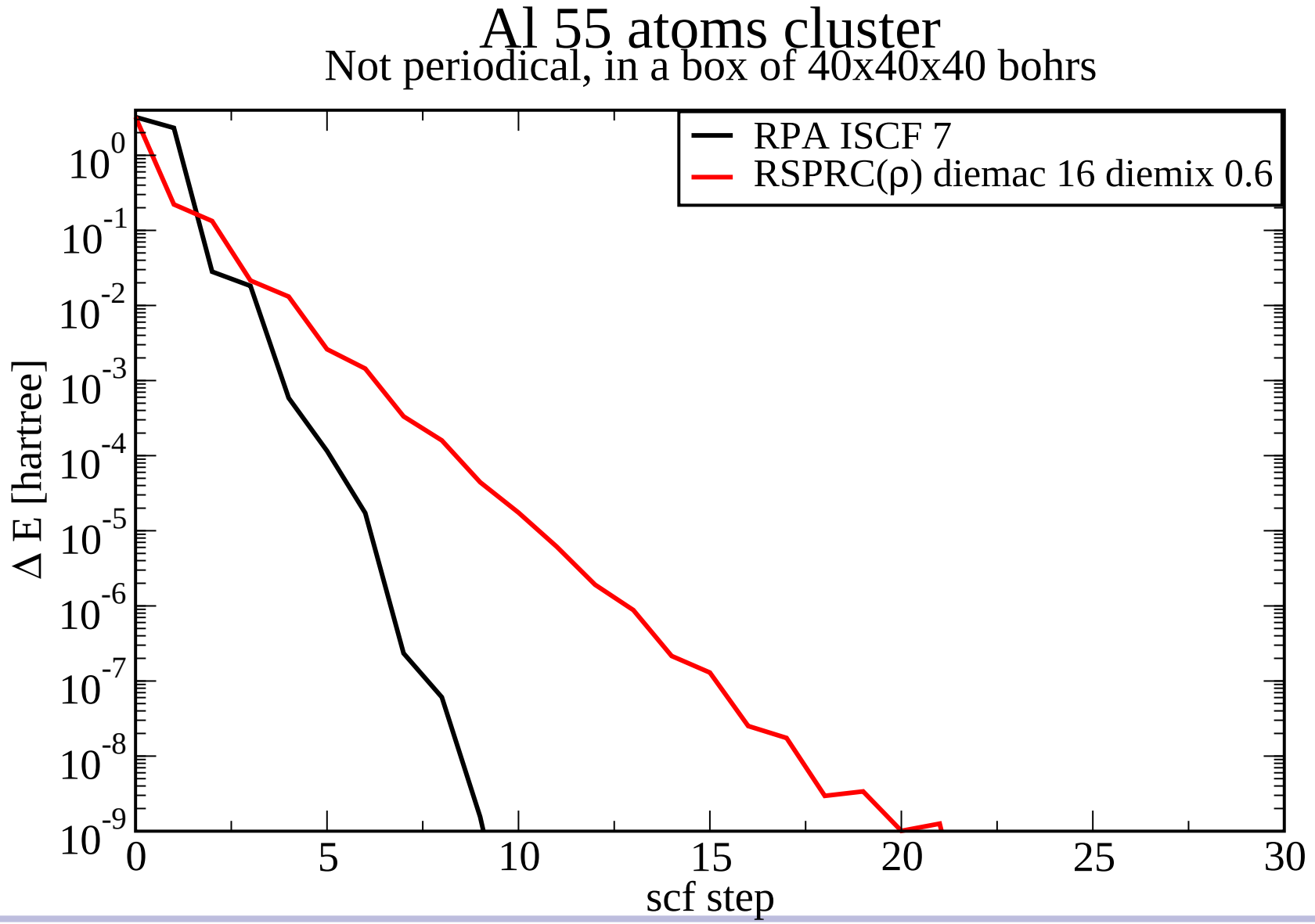

Al 55 atoms cluster
Not periodical, in a box of 40x40x40 bohrs
RPA ISCF 7
RSPRC(ρ) diemac 16 diemix 0.6
Δ E [hartree]
10^0
10^-1
10^-2
10^-3
10^-4
10^-5
10^-6
10^-7
10^-8
10^-9
0
5
10
15
20
25
30
scf step

Table:

	Si $\frac{\text{50\% vacuum}}{\text{50\% bulk}}$			Bulk Si		
type prc	λ_{max}	λ_{min}	CN	λ_{max}	λ_{min}	CN
RPA 24 bands	1.2	0.98	1.2	1.2	0.7	1.7
LDA 61 24 bands	NaN	NaN	NaN	1.2	0.82	1.5
RPA 64 bands	1.1	0.98	1.2	1.1	0.82	1.3
LDA 64 bands	2.3	0.99	2.3	1.2	0.92	1.3
Kerker Diemac 32	2.5	0.18	14	1.5	0.72	2.1
RSKerker Diemac 32	7.3	1.0	7.3	3.9	0.91	4.3
None	31	1.0	31	11	1.0	11