Introduction To The Elk Code

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What is Elk?

- Elk is an all-electron LAPW+l.o. code
- In development for about 8 years (originally the EXCITING code)
- Simple as possible ($\sim 40k$ lines of Fortran 90)
- Aims to be trustworthy
- Aims to be feature-complete
- Aims to be fully documented
- Released under the GPL
- Website: http://elk.sourceforge.net/

Contributors

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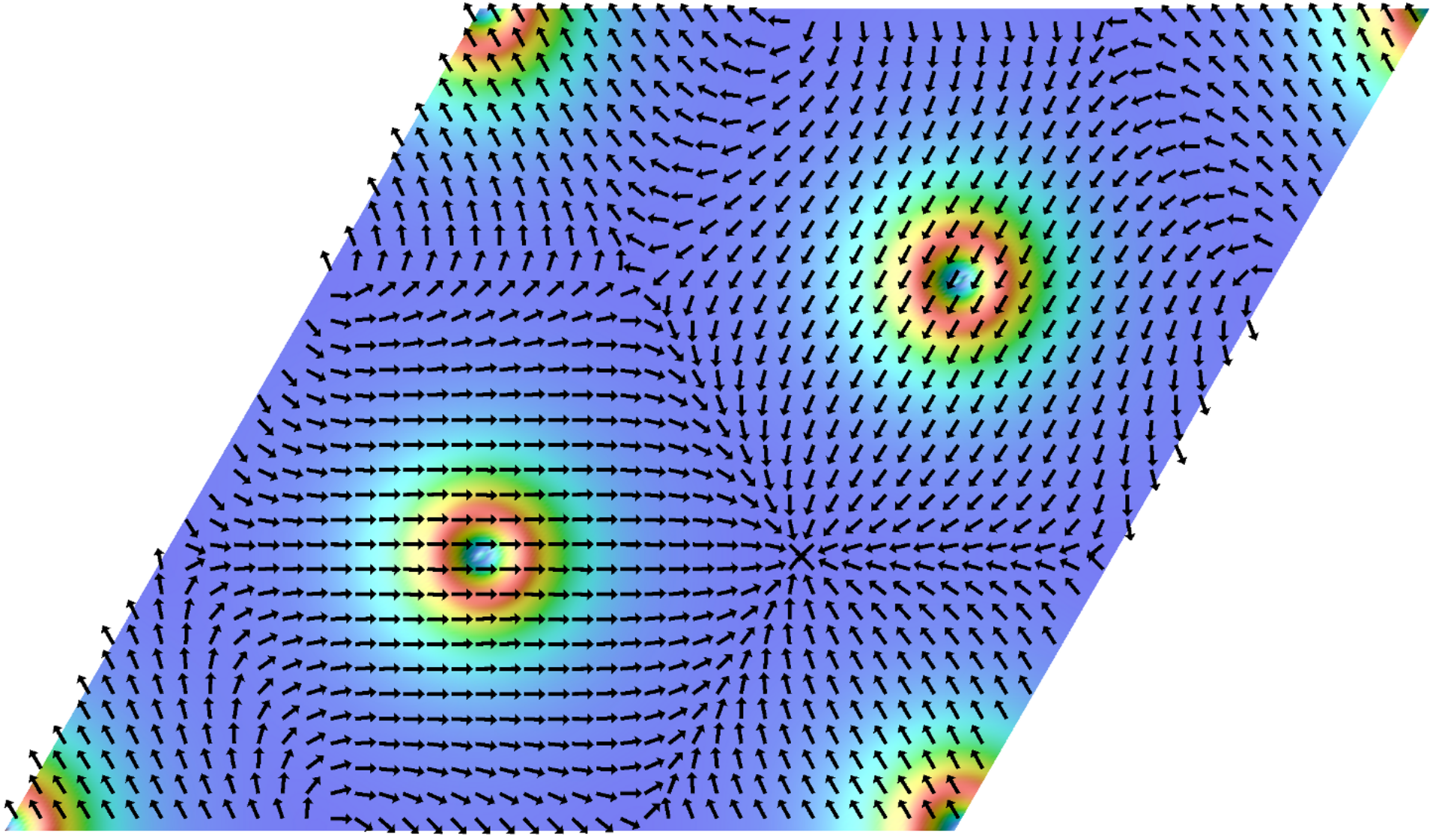
D. J. Singh, *Planewaves, Pseudopotentials and the LAPW Method* (Kluwer Academic Publishers, Boston, 1994)

Features

Basic aim of Elk is to solve the Kohn-Sham equations for external fields

External field	Conjugate field
$V_{\text{ext}}(\mathbf{r})$	$\rho(\mathbf{r})$
$\mathbf{B}_{\text{ext}}(\mathbf{r})$	$\mathbf{m}(\mathbf{r})$
$\mathbf{E}(\mathbf{r})$ $(= -\nabla V(\mathbf{r}))$	$\rho(\mathbf{r})$
$\mathbf{A}$	$\mathbf{j}$

Magnetisation $\mathbf{m}(\mathbf{r})$ of a Cr monolayer



Features

- Kohn-Sham equations solved in two-step process:

  First-variational step: scalar potential and $\mathbf{E}$ only

  $$\hat{H} = \hat{T}_s + \hat{V}_{\text{ext}} + \mathbf{E} \cdot \hat{\mathbf{r}} + \hat{V}_{\text{xc}}$$

  and solve $\hat{H}\phi_i = \epsilon_i \phi_i$

  Second-variational step: add magnetic fields, spin-orbit coupling and $\mathbf{A}$ field

  $$H_{ij} = \varepsilon_i \delta_{ij} + \langle \phi_i | \boldsymbol{\sigma} \cdot (\hat{\mathbf{B}}_{\text{ext}} + \hat{\mathbf{B}}_{\text{xc}}) + \boldsymbol{\sigma} \cdot \hat{L} + \mathbf{A} \cdot \hat{\nabla} | \phi_j \rangle$$

Features

- Full spinor wavefunctions:

$$\phi_{i\mathbf{k}}(\mathbf{r}) = \begin{pmatrix} U^{\uparrow}_{i\mathbf{k}}(\mathbf{r}) \\ U^{\downarrow}_{i\mathbf{k}}(\mathbf{r}) \end{pmatrix} \times e^{i\mathbf{k}\cdot\mathbf{r}}$$

- Spin-spiral states also available:

$$\phi_{i\mathbf{k}}(\mathbf{r}) = \begin{pmatrix} U^{\uparrow}_{i\mathbf{k}}(\mathbf{r}) e^{i(\mathbf{k}+\mathbf{q}/2)\cdot\mathbf{r}} \\ U^{\downarrow}_{i\mathbf{k}}(\mathbf{r}) e^{i(\mathbf{k}-\mathbf{q}/2)\cdot\mathbf{r}} \end{pmatrix}$$

(Frank Essenberger's talk)

Features

- APW radial derivative matching to arbitrary orders at muffin-tin surface
- Arbitrary number of local-orbitals allowed
- LSDA and GGA functions available
- Interface to `libxc`, $>$ 100 functionals (Miguel Marques)
- Fully non-collinear implementation using Kübler's 'trick'
- fixed spin moment or direction
- spin-orbit coupling
- LDA+U available (Lars Nördstrom, Francesco Chricchio)
- Spin-current tensor decomposition (LN, FC)

Features

- Automatic determination of spacegroup symmetry
- Automatic reduction to primitive cell
- Generation of unit cell with spacegroup and Wyckoff coordinates (with `spacegroup` utility)
- Inversion symmetry exploited for real diagonalisation
- Iterative diagonalisation
- Automatic determination and reduction of k-point set
- Symmetrisation of density, potential and fields

Features

- Forces (works with magnetism, etc)
- Structural optimisation
- Various mixing schemes (adaptive, Pulay, Broyden)
- Total DOS, partial DOS in irreducible representations
- Electron localisation function (ELF)
- Electron localisability indicator (ELI) plots with DGrid (Alexey Baranov)
- Plots of wavefunctions, band structures, potentials, etc.
- STM plots

Features

- Core states solved with the Dirac equation
- c is a global constant in the code
- Polarised cores
- Mössbauer isomer shift, EFG and hyperfine fields
- Effective masses
- Fermi surface plots
- Equation of state fitting (with `eos` utility)

Features

- Momentum matrix elements with s.o. correction
- Macroscopic RPA dielectric function
- Kerr angle and Magneto-Optic Kerr Effect (MOKE) output
- Energy loss near edge structure (ELNES) for arbitrary q-vectors
- Non-linear optical (NLO) second-harmonic generation
- Core-state optical spectra (XPS, XAS)

Features

- Hartree-Fock
- Optimised effective potential (OEP) with exact exchange functional
- Reduced density matrix functional theory (RDMFT) (Sangeeta Sharma, Tim Baldseifen, Florian Eich)
- Microscopic RPA function $\epsilon(\mathbf{G}, \mathbf{G}', \mathbf{q}, w)$ in retarded, advance, time-ordered and Matsubara form
- Bethe-Salpeter equation (BSE) beyond Tamm-Dankoff (Matteo Gatti)
- Linear-response time-dependent density functional theory (TDDFT) (SS)

Features

- Phonons for arbitrary **q**-vectors
- Thermodynamic quantities: zero point, free energy, entropy, heat capacity
- Electron-phonon coupling matrices
- Phonon linewidths
- Eliashberg function $\alpha^2 F(\omega)$
- Electron-phonon coupling constant λ
- McMillan-Allen-Dynes superconducting T_c
- Eliashberg equations (Antonio Sanna)

Features

- Everything is interoperable, so you can run:

  A structural optimisation calculation with $\mathbf{A}$, $\mathbf{B}$ and $\mathbf{E}$ fields, in conjunction with a non-collinear, spin-spiral, fixed spin moment, GGA+U calculation, whilst constraining $\nabla \cdot \mathbf{B}_{\mathrm{xc}} = 0$, and then compute a BSE core-state spectra beyond the Tamm-Dankoff approximation on top of this.

  This interoperability makes for robust code

Limitations

Can't (yet) perform

- Molecular dynamics
- Automatic stress/strain/elastic tensor
- Automatic isobaric/isovolumetric optimisation
- *GW* approximation
- Dynamical mean field theory (DMFT)
- Superconducting density functional theory (SCDFT)
- True non-collinear functional for spin-dynamics (F. Eich)
- TDDFT in real-time for attosecond electron dynamics
- Berry phase
- Meta-GGA and van der Waals functionals
- ...

Requirements

Minimum requirements:

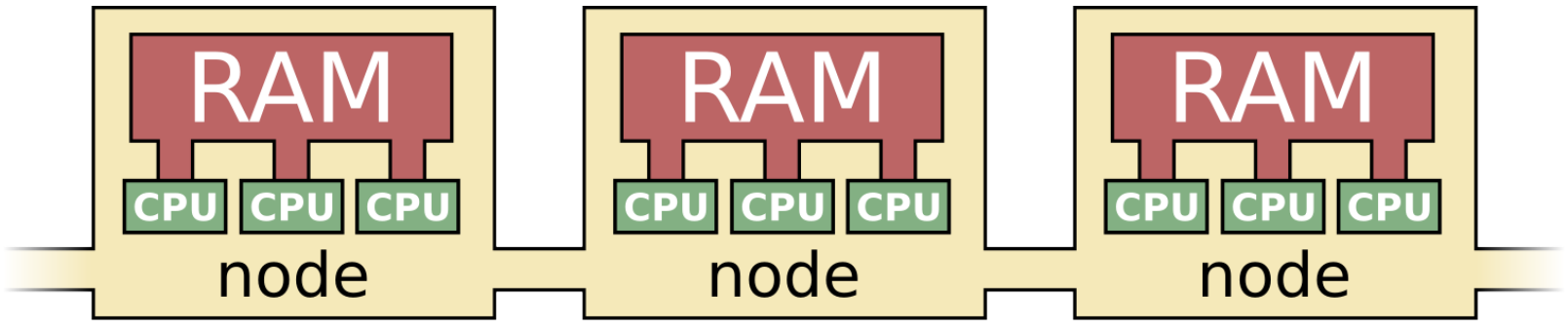
- UNIX/Linux based computer
- Optimising Fortran 90 compiler

Recommended requirements:

- Multi-node computer cluster
- OpenMP + Message Passing Interface (MPI) environment
- Optimised BLAS/LAPACK and FFT libraries

Parallelism in Elk

Parallelism in Elk



Memory bus

Bandwidth: ~35 GB/s

Latency: ~10 ns

Infiniband

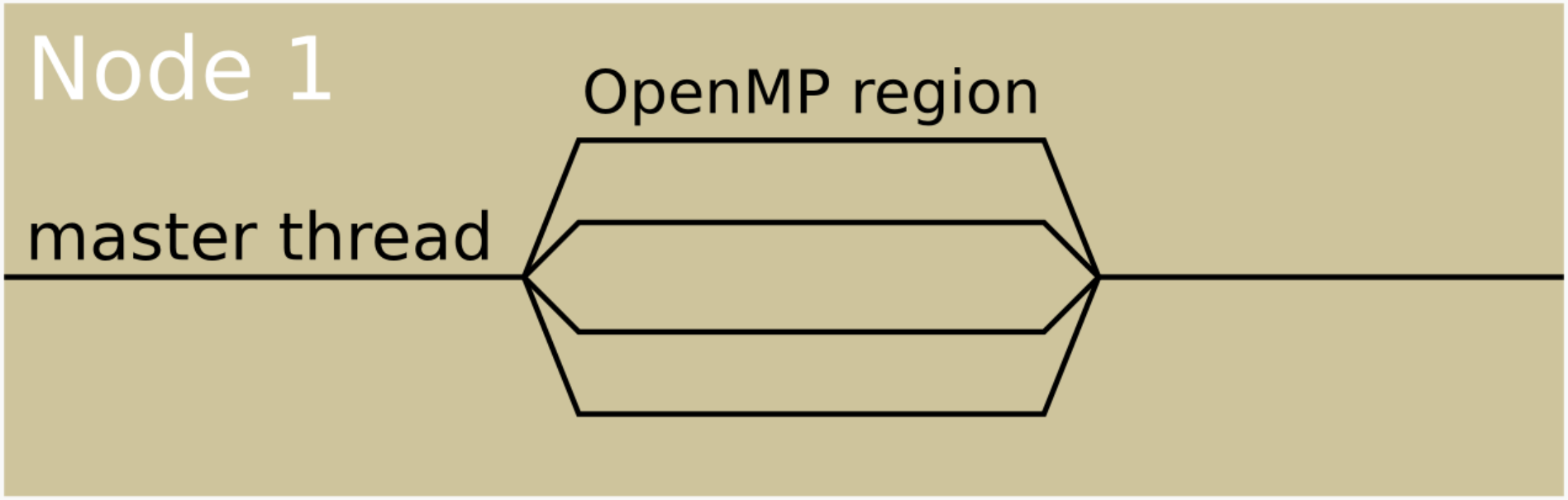
Bandwidth: 1-5 GB/s

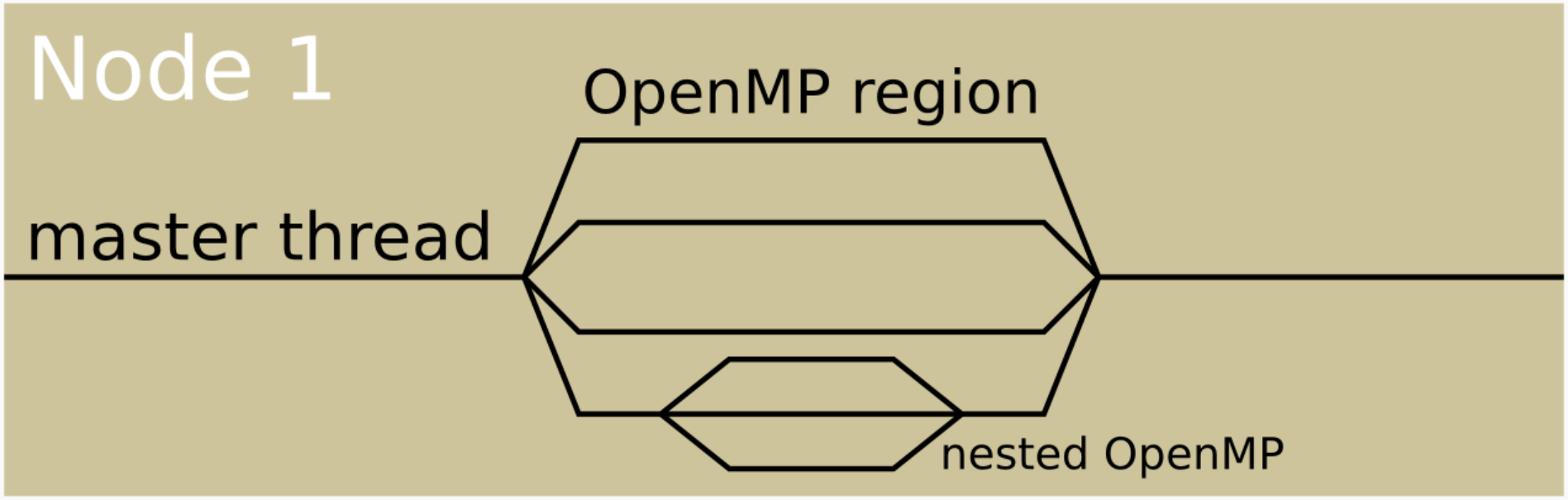
Latency: ~1 µs

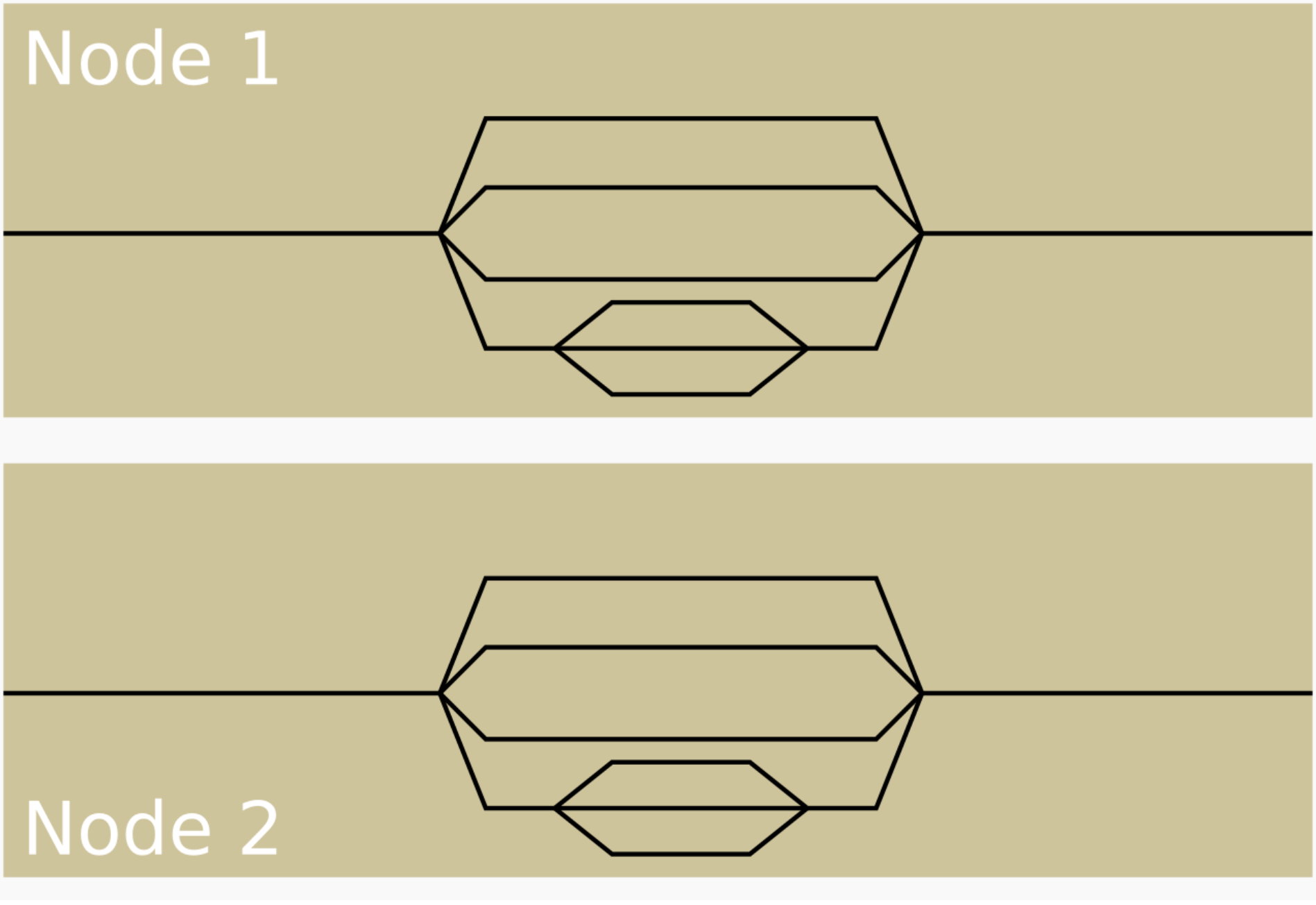
Parallelism in Elk

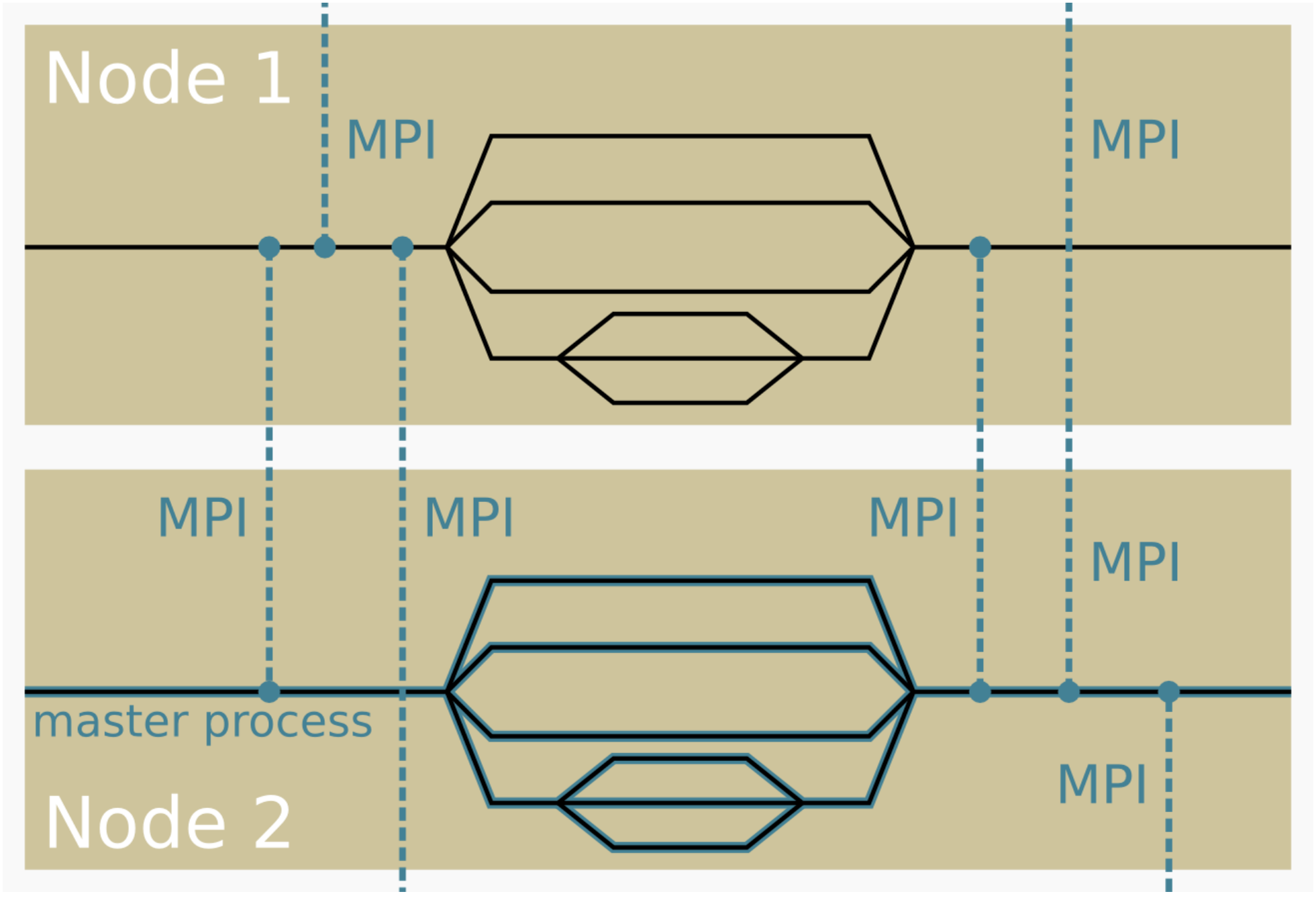
Code parallelised in three ways:

- OpenMP
  (also in MKL/ACML BLAS/LAPACK/FFT libraries)
- Message Passing Interface (MPI)
- Phonon calculations via networked filesystem


Node 1
OpenMP region
master thread


Node 1
OpenMP region
master thread
nested OpenMP


Node 1
Node 2


Node 1
MPI
MPI
MPI
MPI
MPI
MPI
MPI
master process
Node 2

- Parallelised over k-points with MPI and OpenMP
- Parallelised over states, atoms, $\mathbf{G}$-vectors with OpenMP
- Parallelised over q-points, atoms and polarisations for phonon calculations with NFS
- BLAS/LAPACK/FFT parallelised with MKL/ACML

Compiling Elk

1. Download and unpack `elk-1.3.24.tgz`
2. Run `setup`
3. Edit `make.inc` for optimimal performance
4. Run `make`

The executable is `elk` and in the directory `elk/src/`

Running Elk

Normally, only one input file is required: `elk.in`

All output files are in uppercase and have the extension `.OUT`
Some are binary, others are human-readable

General information in the file `INFO.OUT`

Elk.in

```
tasks
  0   :  ground-state run
  10  :  total and partial DOS
  120 :  momentum matrix elements
  180 :  RPA ϵ^{-1}(G, G', q, w)
  185 :  Bethe-Salpeter equation (BSE)

avec
  5.13 5.13 0.00
  5.13 0.00 5.13
  0.00 5.13 5.13

atoms
  1
  'Si.in'
  2
  0.0 0.0 0.0
  0.25 0.25 0.25

ngridk
  5 5 5
```

Species files

Species files are required to tell the code things like muffin-tin radius, type of (L)APW, local-orbitals and which states are in the core

Elements from H to Rf available in the `elk/species/` directory

Running Elk

Full test suite, just run

```
make test
```

Wide range of examples available in `elk/examples/` which demonstrate many features of the code

Also available is the Elk manual and a very active forum on the Elk website

Units

All input and output units are atomic: Units obtained by setting

$$m_e = 1 \qquad e = 1 \qquad \hbar = 1 \qquad 4\pi\epsilon_0 = 1$$

Dervied units:

- Length: 1 Bohr $a_0 = 4\pi\epsilon_0/m_e e^2 \sim 0.52918$ Å
- Energy: 1 Hartree $E_H = m_e e^4/(4\pi\epsilon_0\hbar)^2 \sim 27.211$ eV
- Time: $\hbar/E_h \sim 2.418 \times 10^{-17}$ s
- Magnetic field: $e/a_0^2 \sim 1715.255$ Tesla

Also note $\alpha = e^2/(4\pi\epsilon_0)\hbar c$, thus

$$c = \frac{1}{\alpha} \sim 1/137$$

Globally adjustable in Elk

Beware

It's easy to generate rubbish with electronic structure codes

Always check for convergence with respect to relevant variables:

- `rgkmax`: planewave cut-off for APWs
- `lmaxapw`, `lmaxvr`, `lmaxmat`: angular momentum cut-offs
- `nempty`: number of first-variational states, and therefore second-variational basis size
  (essential for magnetism, optics, ...)
- `ngridk`: k-point grid
- ...

Also compare with other codes: ABINIT, VASP, PWSCF, Wien2k, EXCITING, FLEUR, RSPt, SIESTA, CASTEP, etc.