JÜLICH
FORSCHUNGSZENTRUM

Condensed Matter Codes

Potential Application of Active Storage

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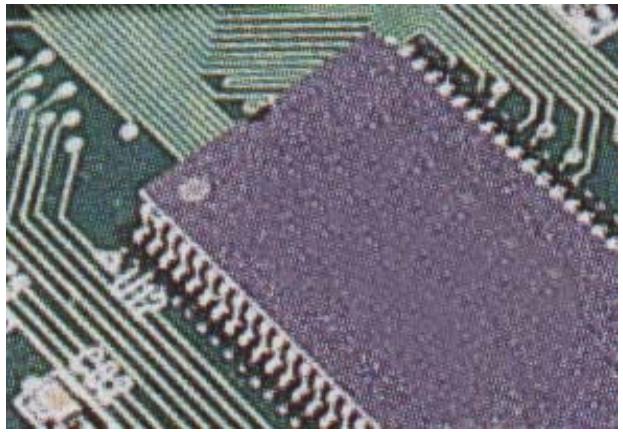
Describing Electrons in Solids and Molecules

This encompasses

- Half of Chemistry
- Half of Condensed Matter Physics
- Most of Nanoscience
- Large part of Materials Science
- Smaller part of Life Science

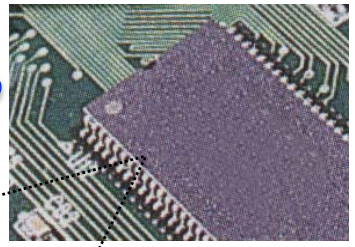


No surprise, such problems have a share of about 50% at computer centers in the world

Matter – Materials – Device

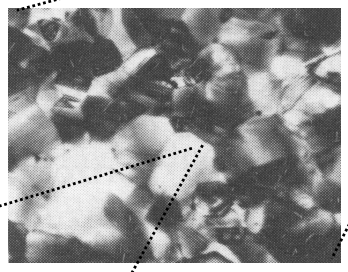
from materials
to device

from matter
to materials



MACRO

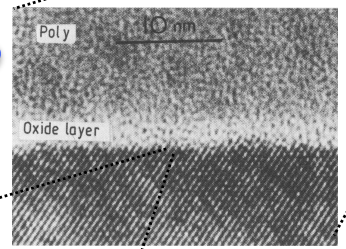
10^{-2}m, 10^{8}s



MESO

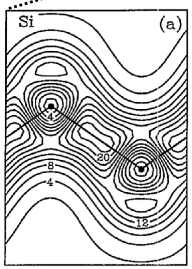
10^{-6}m, 10^{0}s

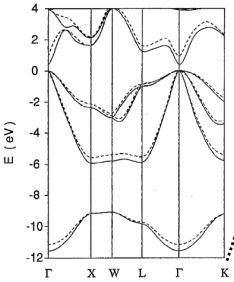
10 nm



ATOMS

10^{-9}m, 10^{-12}s



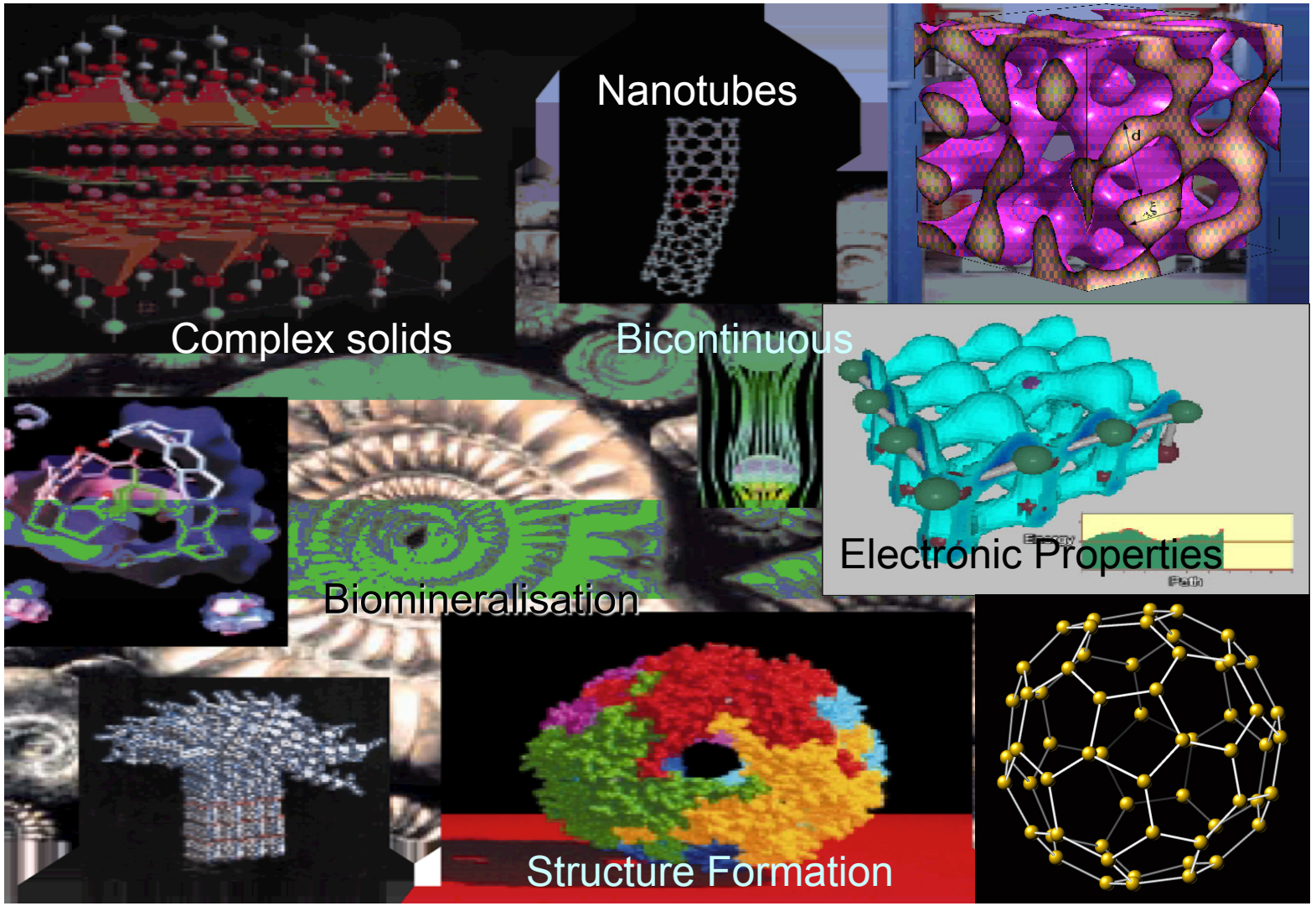


ELECTRONS

10^{-10}m, 10^{-15}s

courtesy of
materialscience.com

Huge Complexity



Quantum Mechanics of Electrons

$$H = -\frac{\hbar^2}{2m}\sum_{j=1}^{N_e}\nabla_j^2 - \sum_{\alpha=1}^{N_i}\frac{\hbar^2}{2M_\alpha}\nabla_\alpha^2 - \sum_{j}^{N_e}\sum_{\alpha=1}^{N_i}\frac{Z_\alpha e^2}{|r_j - R_\alpha|} + \sum_{j<k}^{N_e}\frac{e^2}{|r_j - r_k|} + \sum_{\alpha<\beta}^{N_i}\frac{Z_\alpha Z_\beta e^2}{|R_\alpha - R_\beta|}$$

Schrödinger & Dirac (1929)

- Basic equations are known
- But unsolvable many-body problem

Example: 1 iron atom / unit cell

26 electron wave-function: $\Psi(r_1,\ldots r_{26})$

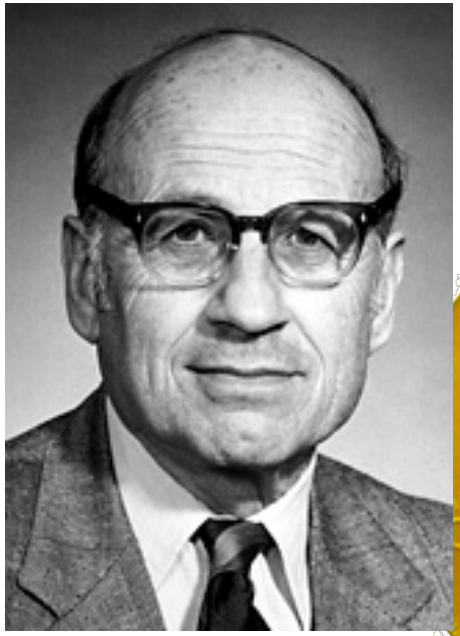
store only 10 values per coordinate: 10^{78} values

assume each value could be stored in a single H atom:

memory heavier than the milky way

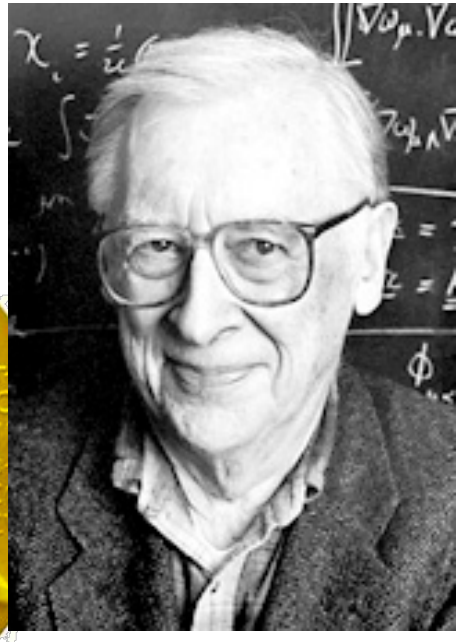
The Nobel Prize in Chemistry 1998

"for his development of the density-functional theory"



Walter Kohn

"for his development of computational methods in quantum chemistry"

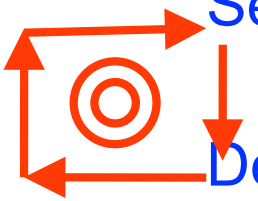


John A. Pople

The Kohn-Sham Standard Model

"**The** Computational Approach" for
Physics, Chemistry, Nanoscience, Materials Science, Mineralogy, Geology, …

Total energy $E_{\text{total}} = E[n(\mathbf{r}), a_0, \{\mathbf{R}_a\}, \mathbf{m}(\mathbf{r}), \ldots]$
is functional of electron density n and external parameters such as lattice constants a_0, atoms positions $\mathbf{R}_a$, magnetization direction $\mathbf{m}$, …



Secular equation $\hat{H}[n]\Psi_i[n](\mathbf{r}) = \varepsilon_i[n]\Psi_i[n](\mathbf{r})$

Selfconsistency loop

Density $n(\mathbf{r}) = \sum_i^{\text{occup.}} |\Psi_i(\mathbf{r})|^2$

CPU-Time scaling ~ $N_{\text{atoms}}{}^3 \approx \text{Volume}^3, \approx \text{Precision}^3$

The Kohn-Sham Standard Model

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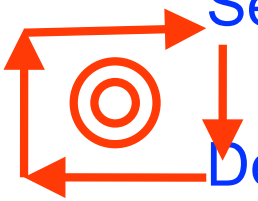


Secular equation $\hat{H}[n]\Psi_i[n](\mathbf{r}) = \varepsilon_i[n]\Psi_i[n](\mathbf{r})$

Selfconsistency loop

Density $n(\mathbf{r}) = \sum_{i}^{\text{occup.}} |\Psi_i(\mathbf{r})|^2$

Memory scaling

i~ N_{atoms} & **r** ~ N_{atoms} ➔ Volume^2

General Algorithm

Molecular Dynamics ~1000 real-time steps or
Geometry relaxation ~10-30 steps

Electronic self-consistency of $n(\mathbf{r})$ ~15-100 steps

$$E_{\text{tot}}[n] = E_{\text{kin}}[n] + E_{\text{ext}}[n] + E_{\text{H}}[n] + E_{\text{xc}}[n]$$

Setup of Secular Equation
Solve Secular Equation

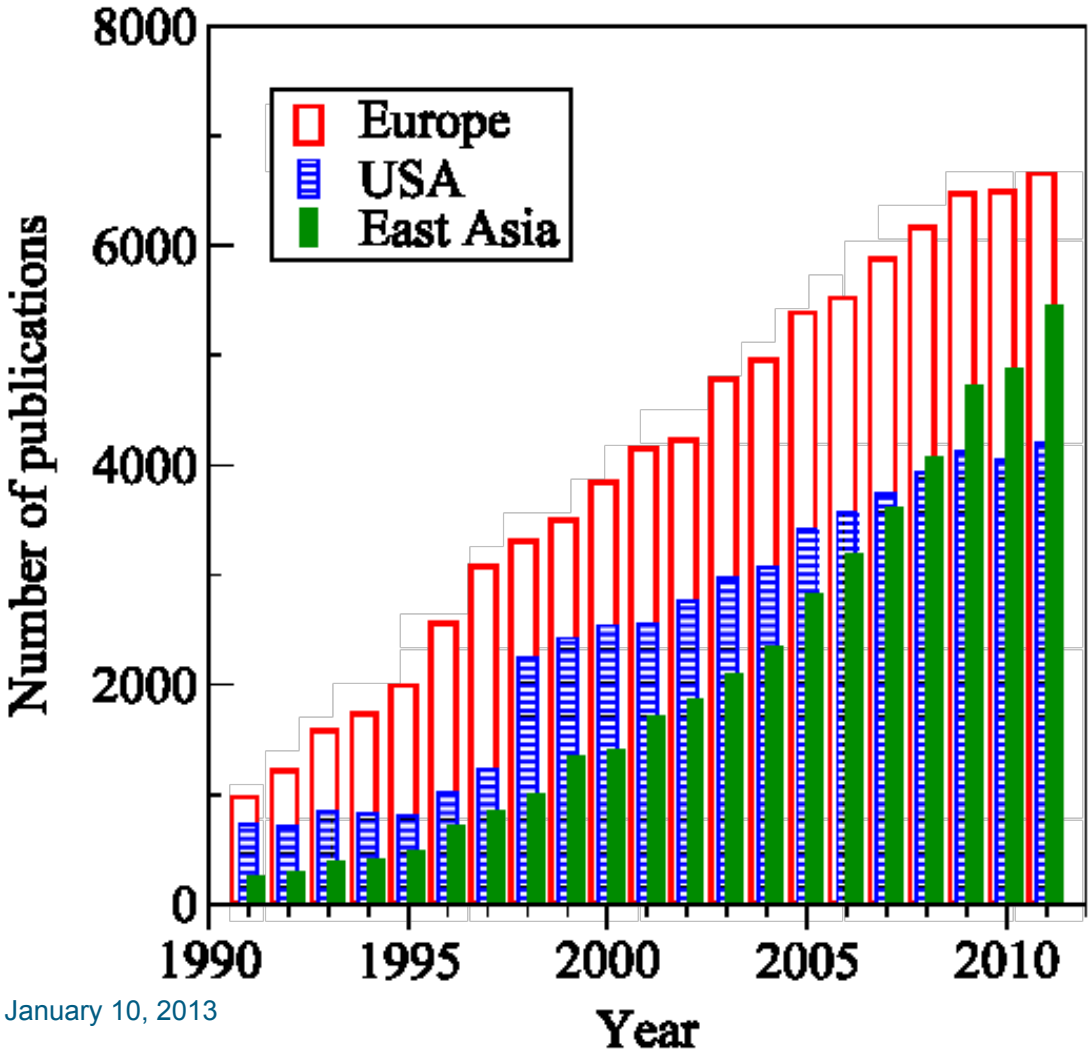
That's where the CPU time goes!

electronic eigenstates
electronic density $n(\mathbf{r})$
and ionic forces $\mathbf{F}_a = -\frac{\partial}{\partial \mathbf{R}_a}\left(E[n] + E_{\text{ion-ion}}\right)$

Minimum of Total Energy

$$t_{\text{CPU}} \approx N_{\text{MD}} N_{\text{iter}} N_{\text{atoms}}^{\ 3}$$

Publication of DFT results/year



DFT-calculations became a huge international enterprise reaching 17.000 publications a year

There is a crowd!

Analysis: Web of Science
Key words:
- First-principles
- Ab initio
- Density functional

Density Functional Methods

- full-relativistic
- scalar-relativistic
- non-relativistic

- local density approximation (LDA)
- generalized gradient approx. (GGA)
- spin integrated
- spin polarized / non-collinear spin
- LDA+U, OEP
- hybrid functionals
- current density functional

- **Real-Space grid**
- Plane Waves
- Non-linear methods
  - AugmentedPW
  - **KKR-GF**
- Linearized methods
  - LinearizedAPW
  - ASW
  - LMTO
- Linear Combination of Atomic Orbitals
  - tight-binding
  - Gaussian Os
  - Slater type Os
  - numerical AOs
- …

$$\left[\frac{\hat{\mathbf{p}}^2}{2m_e} + V_{\text{ion}}[\{\mathbf{R}_a\}](\mathbf{r}) + V_{\text{Hxc}}[n](\mathbf{r})\right]\Psi_i(\mathbf{r}) = \varepsilon_i\Psi_i(\mathbf{r})$$

- non-periodic
- periodic
- symmetrized
- real-space

- all electrons, full potential
- all electrons, spherical pot.
- pseudopotential (valence e^-)
- jellium approx. (no structure)

Three Aspects of Bandstructure Methods

Efficient solution of the (generalized) eigenvalue problem

$$\sum_j \left(H_{ij}[\{\mathbf{R}_\mathrm{a}\}, n] - \varepsilon S_{ij}[\{\mathbf{R}_\mathrm{a}\}] \right) \chi_j = 0$$

➔ Very efficient basis set (small number per atom)

➔ Basis set, which lead to specialized matrices (fast algorithm)

You have to think about {
- o Geometrical model
- o What kind of electrons to treat
- o Basis sets

Outline

Density Functional Theory
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RealSpace
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juRS

MultipleScattering
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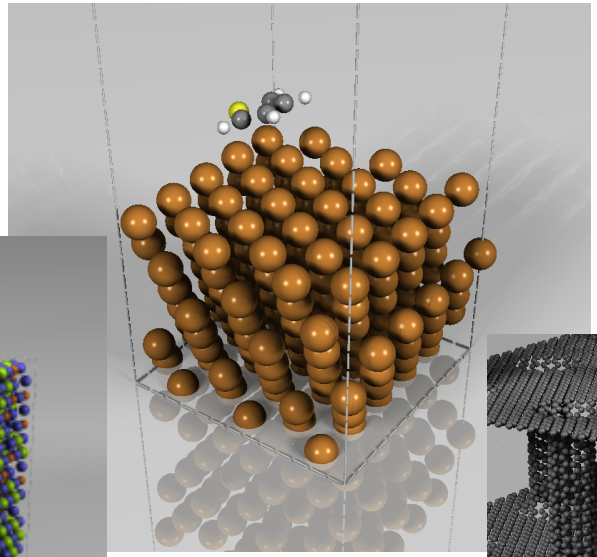
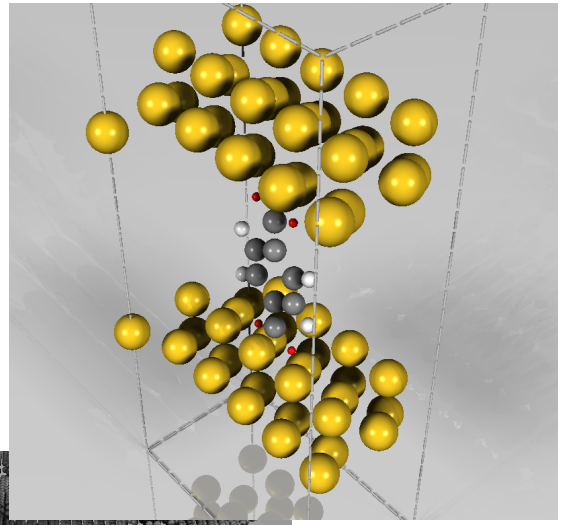
KKRnano

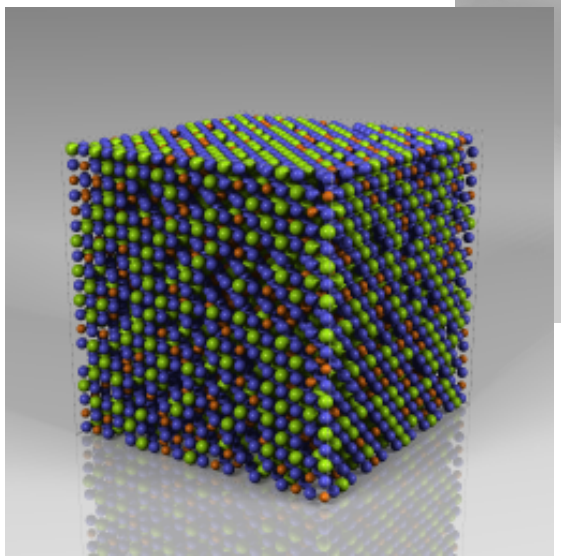
Application of jüRS

Molecules on surfaces

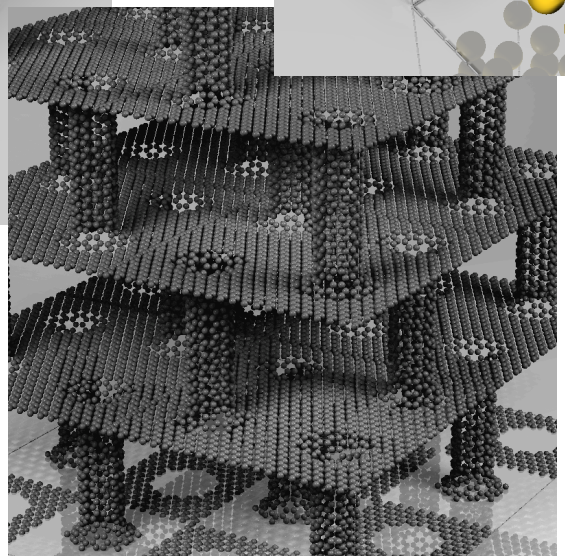


STM situations





Phase-Change materials
Disorder & localization



Graphene and derivatives

Ge

Uniform Real-Space Grid

grid spacing h → real-space vector $\vec{r}_{\vec{i}} = \vec{i}h$

$$\left(-\frac{1}{2}\Delta + V(\vec{r}) - E\right)\Psi(\vec{r}) = 0$$

KineticEnergy LocalPotential EnergyEigenvalue

$$\left(-\frac{1}{2}\Delta_{\mathrm{FD}} + V(\vec{r}_i) - E\right)\Psi(\vec{r}_i) = 0$$

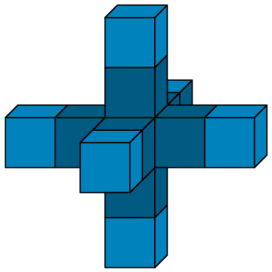
finite-difference derivative

Uniform Real-Space Grid

grid spacing h → real-space vector $\vec{r}_{\vec{i}} = \vec{i}h$

$$\left(-\frac{1}{2}\Delta + V(\vec{r}) - E\right)\Psi(\vec{r}) = 0$$

KineticEnergy LocalPotential EnergyEigenvalue

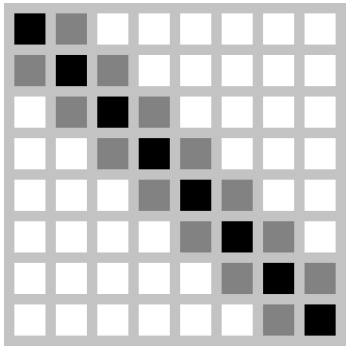


4th order stencil in 3D

$$\left(-\frac{1}{2}\Delta_{FD} + V(\vec{r}_i) - E\right)\Psi(\vec{r}_i) = 0$$

finite-difference derivative (2nd order in 1D)

matrix scheme
2nd order in 1D



$$\Psi_i'' = \frac{1}{h^2}\left(\Psi_{i-1} - 2\Psi_i + \Psi_{i+1}\right)$$

choose periodic or isolated boundary condition

Parallelization of the KS-equation

solving the KS-equation needs most of the time

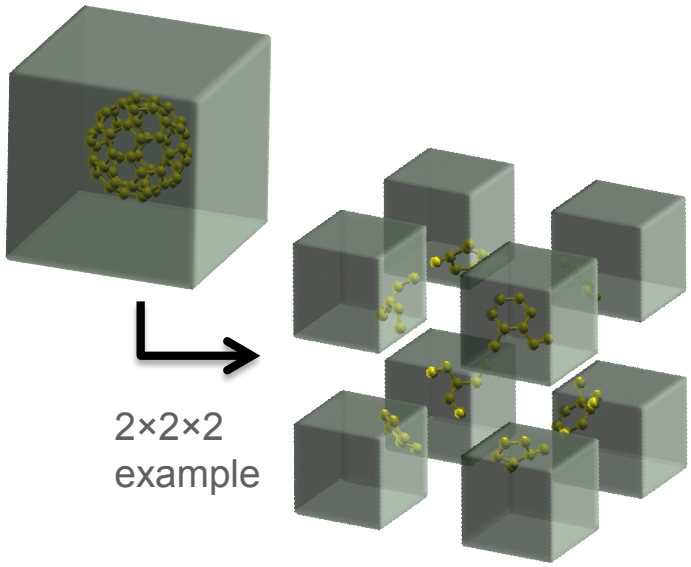
$$\left[\hat{H}_{\sigma\vec{k}} - \epsilon_{n\sigma\vec{k}}\hat{S}_{\vec{k}}\right]\Psi_{n\sigma\vec{k}}(x,y,z) = 0$$

three levels of parallelization

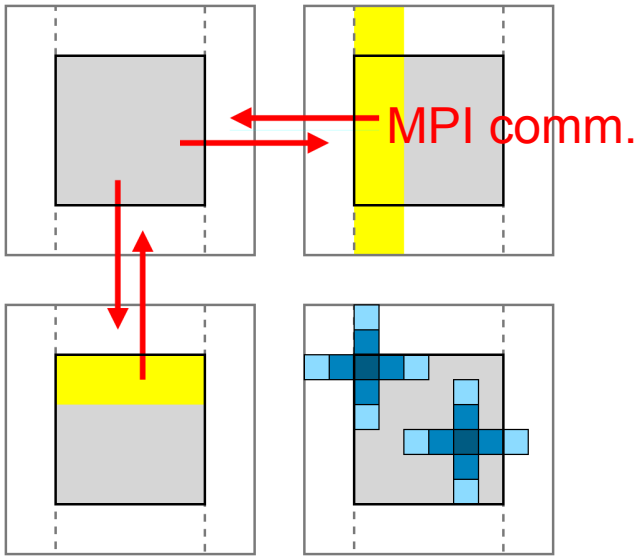
- $\underline{k}$-points and spins σ
- real-space grid x, y, z
- eigenstates/bands n

Distribute the Real-Space Grid: Domains

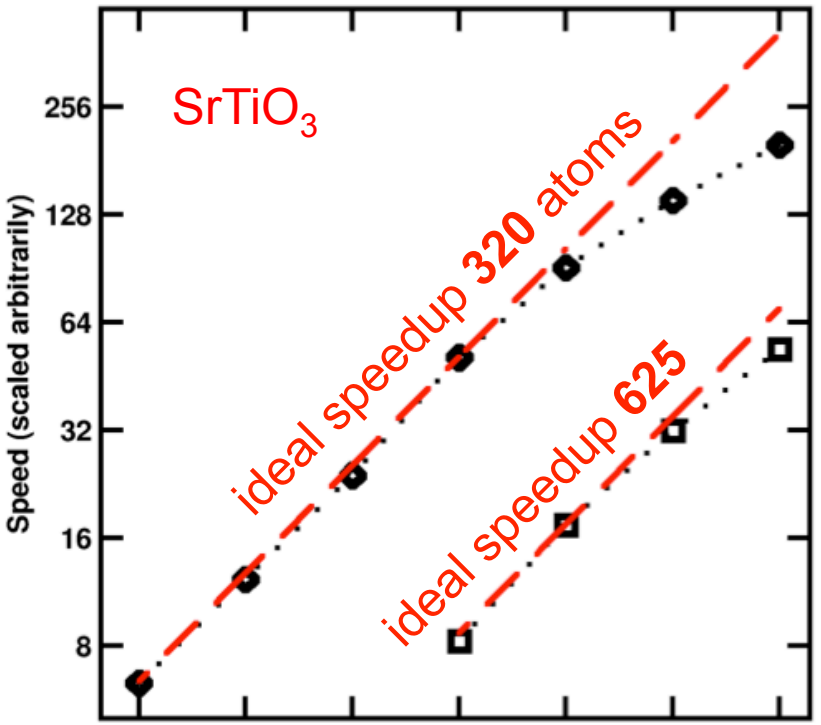
the total number of grid points
is distributed equally among
$N_x \times N_y \times N_z$ processes



exploit data locality:
the finite-difference-Hamiltonian
allows a restriction to Cartesian
nearest-neighbor communications



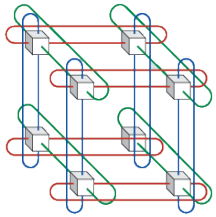
Grid Parallelization in Domain Decomposition

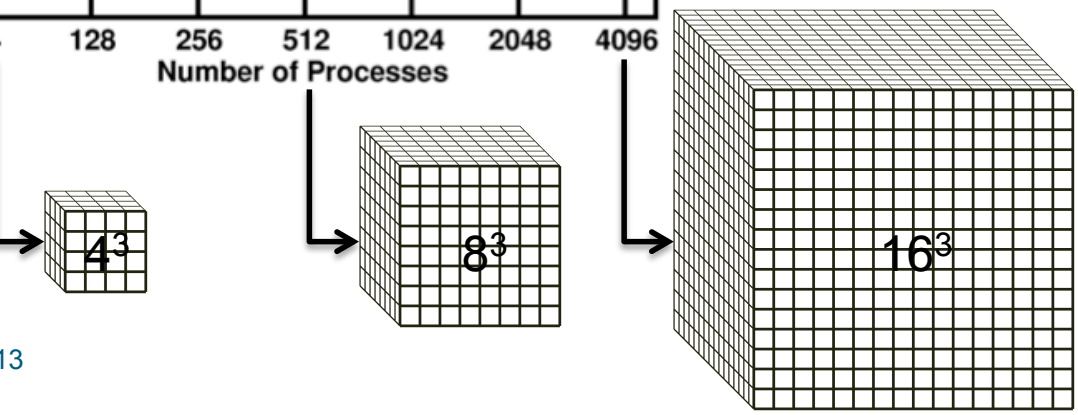


hard scaling

$\Psi(x, y, z)$

torus network





juRS - I/O profile

Minimal Input, master reads and broadcasts
atomic coordinates $\mathbf{R}_a$ and one file (500 kByte) per species

Log output (ASCII) by master

Parallel output of density and wave functions Ψ at the end
single file ~ 64 kByte × N_{atoms}^2
MPI I/O times < 1%

$$\Psi_{n\sigma\vec{k}}(x, y, z)$$

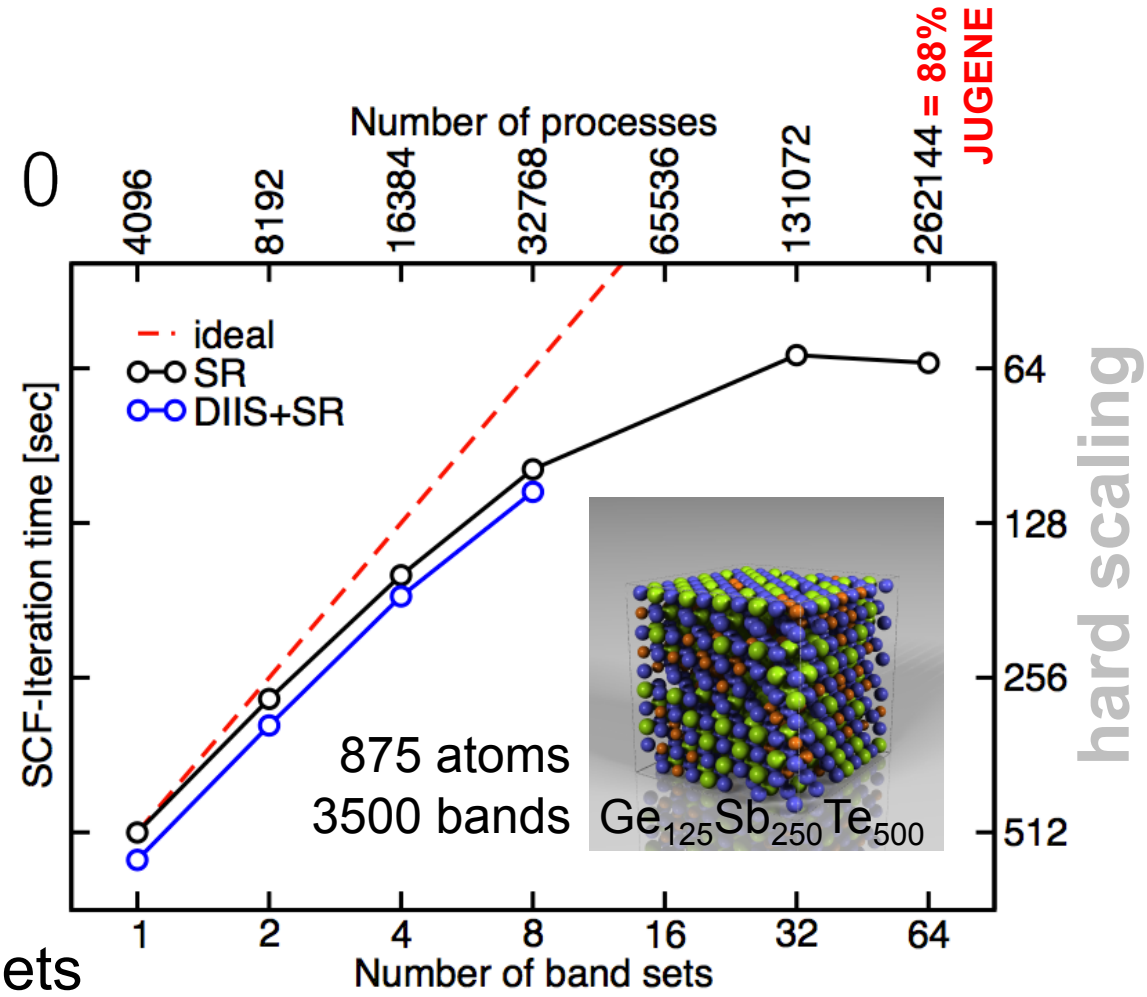
1 TByte for 4000 atoms

in MD calculations:
ⓘ Active Storage for checkpointing of Ψ replacing FS I/O

Band Parallelization

$$\left[\hat{H} - \epsilon_n \hat{S}\right] \Psi_n(\vec{r}) = 0$$

$\Psi_{n\sigma}$



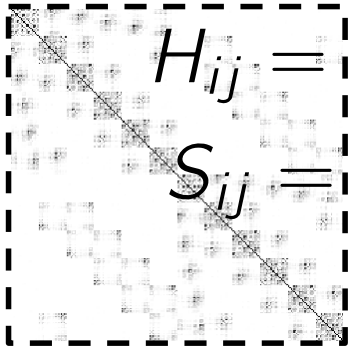
no data locality

solves memory issue

➔ acceleration up to 32 sets

Subspace Solver

① Setup of the subspace matrices



$$H_{ij} = \langle \Psi_i | \hat{H} | \Psi_j \rangle$$
$$S_{ij} = \langle \Psi_i | \hat{S} | \Psi_j \rangle$$

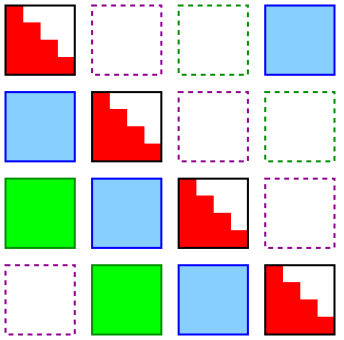
② Solve the generalized eigenvalue problem in the subspace $H_{ij}\Phi_{jn} = \epsilon_n S_{ij}\Phi_{jn}$

③ Apply new linear combination to states $|\Psi'_k\rangle = \Phi_{kj} |\Psi_j\rangle$

Subspace Solver with Band Parallelization

① Setup of the subspace matrices
+MPI communication

$$H_{ij} = \langle \Psi_i | \hat{H} | \Psi_j \rangle$$
$$S_{ij} = \langle \Psi_i | \hat{S} | \Psi_j \rangle$$

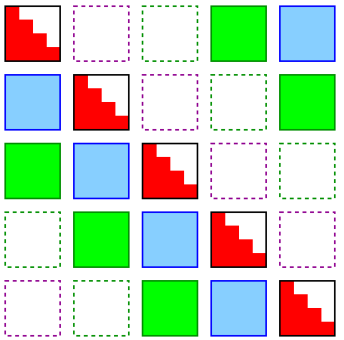


$N_{\text{tasks}} = 4$

② Solve the generalized eigenvalue problem in the subspace $H_{ij}\Phi_{jn} = \epsilon_n S_{ij}\Phi_{jn}$

③ Apply new linear combination to states
+MPI communication

$$|\Psi'_k\rangle = \Phi_{kj} |\Psi_j\rangle$$



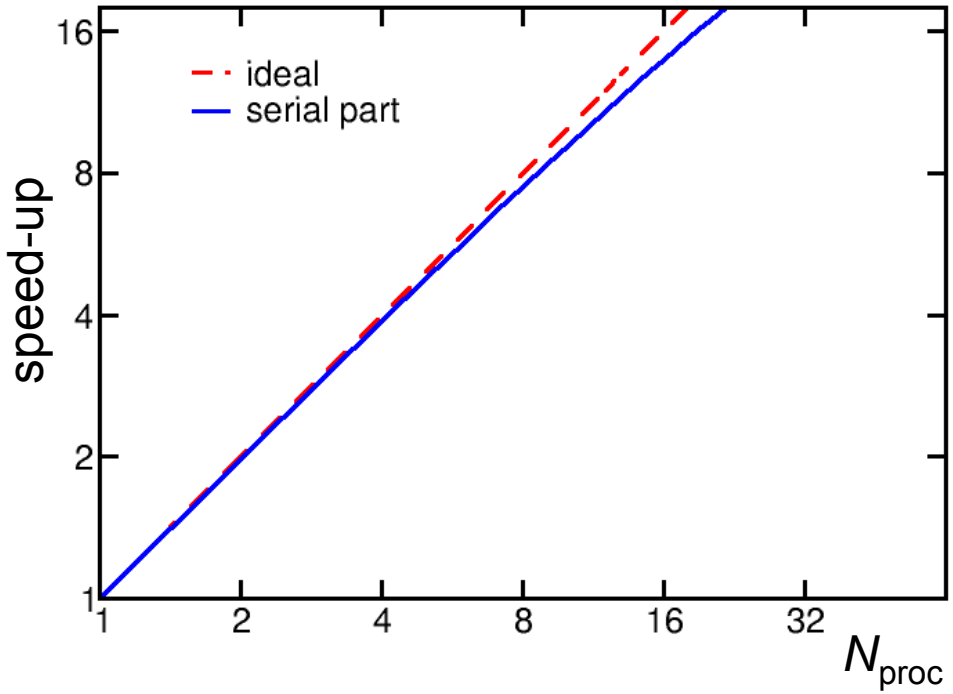
$N_{\text{tasks}} = 5$

Application of Active Storage

SubspaceRotation time $t_{execution}(N_{proc})$

+ parallelizable part ~$1/N_{proc}$
+ serial fraction ~ const

Speed-up = $t_{exec}(1)/t_{exec}(N_{proc})$

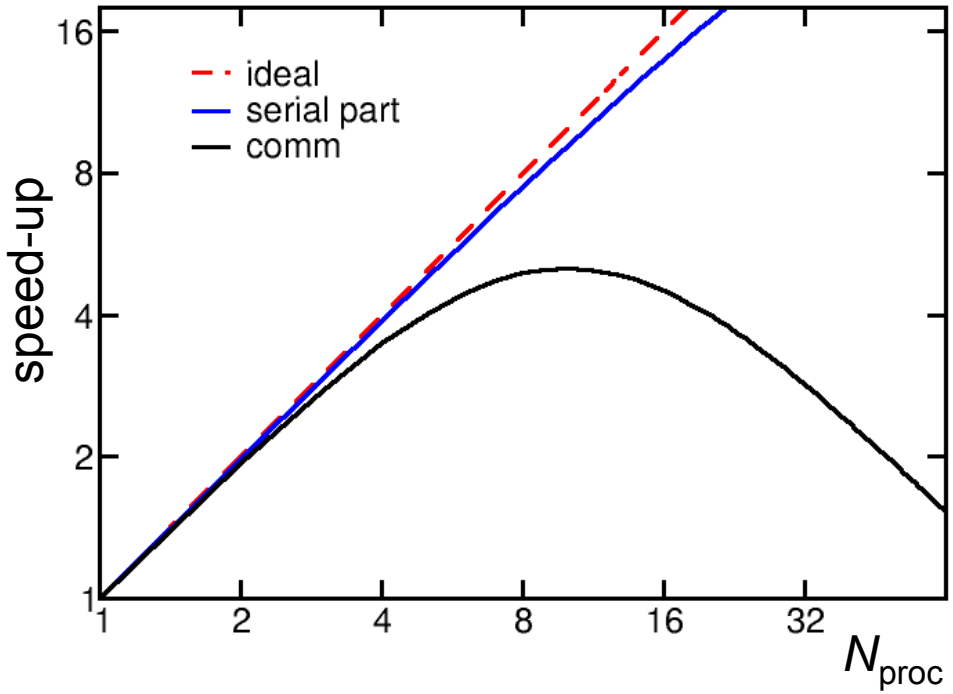


Application of Active Storage

SubspaceRotation time $t_{execution}(N_{proc})$

+ parallelizable part ~$1/N_{proc}$
+ serial fraction ~ const
+ communication ~$(N_{proc}-1)$

Speed-up = $t_{exec}(1)/t_{exec}(N_{proc})$

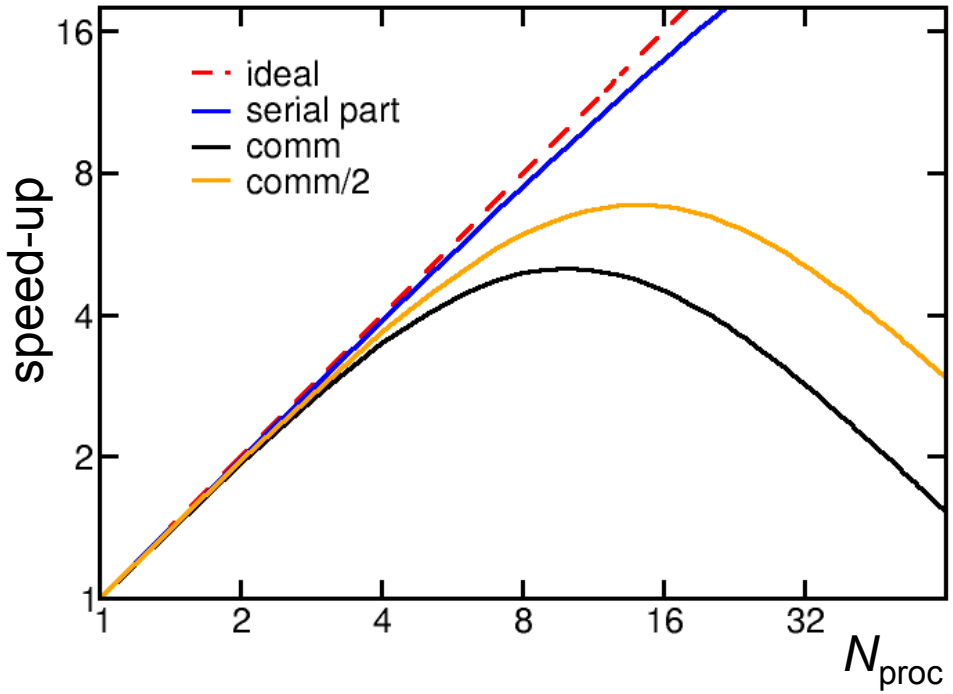


Application of Active Storage

SubspaceRotation time $t_{execution}(N_{proc})$

+ parallelizable part ~$1/N_{proc}$
+ serial fraction ~ const
+ communication ~$(N_{proc}-1)$

Speed-up = $t_{exec}(1)/t_{exec}(N_{proc})$



ⓘ store “remote” wave functions after the initial communication in ActiveStorage and re-use them for the new linear combination

➔ reduce the prefactor for communication by 2 (accepting ASI/O)

Outline

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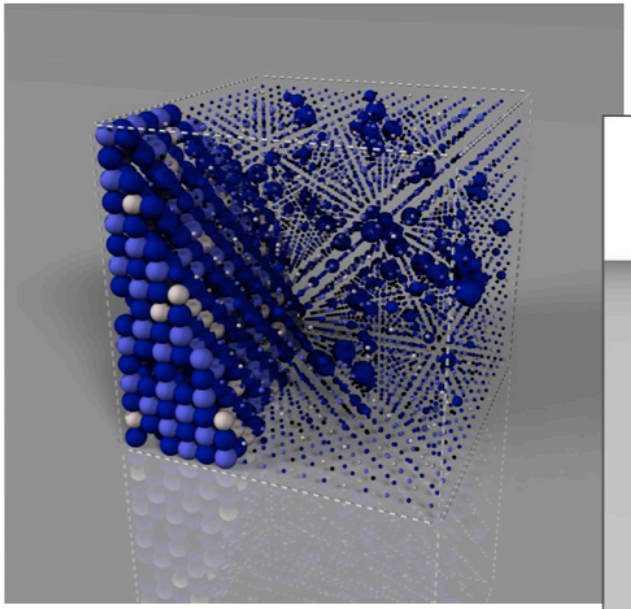
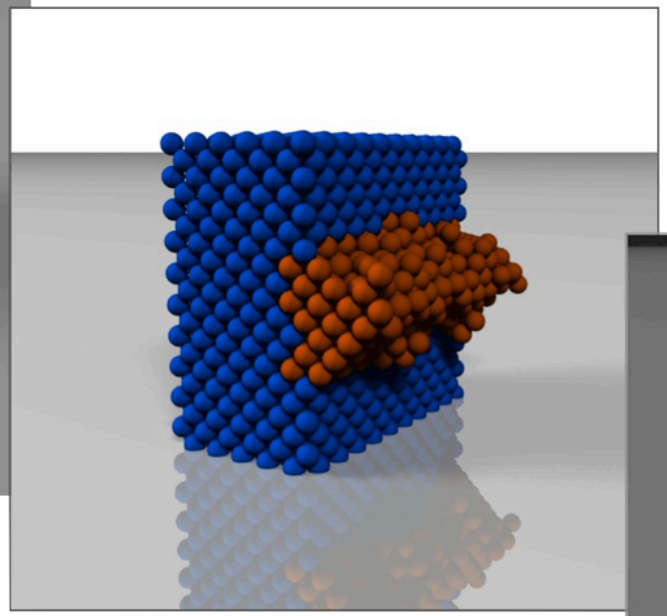
RealSpace juRS
p.baumeister@fz-juelich.de

MultipleScattering KKRnano
ru.zeller@fz-juelich.de

Application of KKRnano

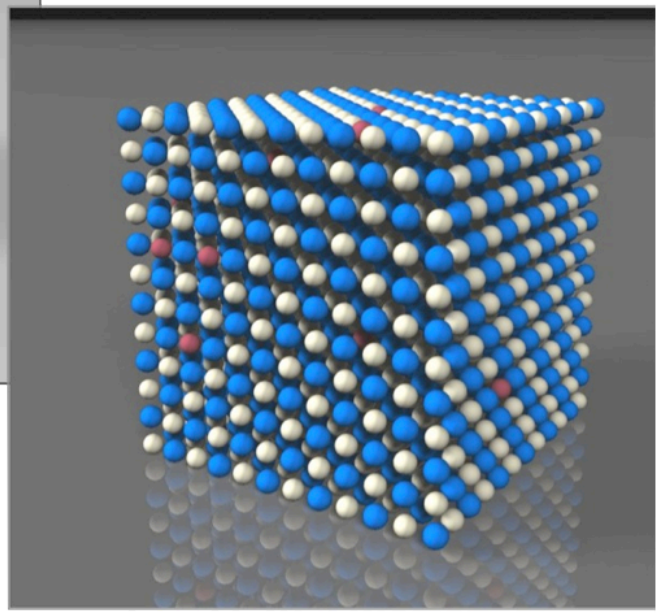


Phase-Change Materials
GeSbTe disorder & localization



Magnetic Metallic Compounds
Fe_xCo_{1-x} magnetic exchange
Ni in Pd induced moments
Cu in Ni Konbu-phase

Dilute Magnetic Semiconductors
MgO:N magnetic exchange
GaN:Gd colossal moments



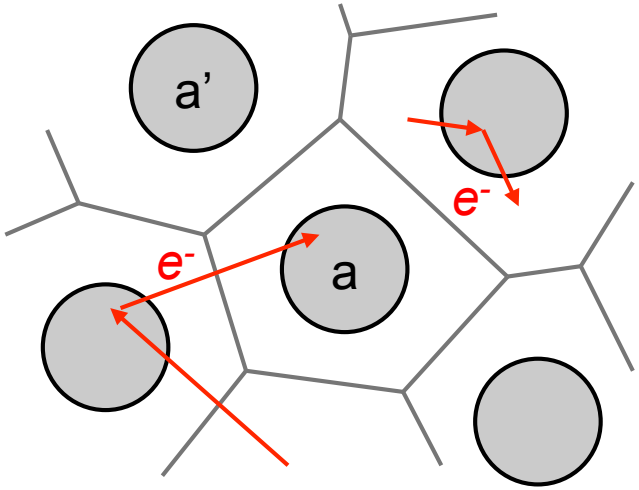
KKRnano: Inversion of huge sparse matrices

Multiple-Scattering theory

$$n(\mathbf{r}) = -\frac{1}{\pi}\Im \int_{-\infty}^{E_F} \mathrm{d}E\, G(\mathbf{r},\mathbf{r},E)$$

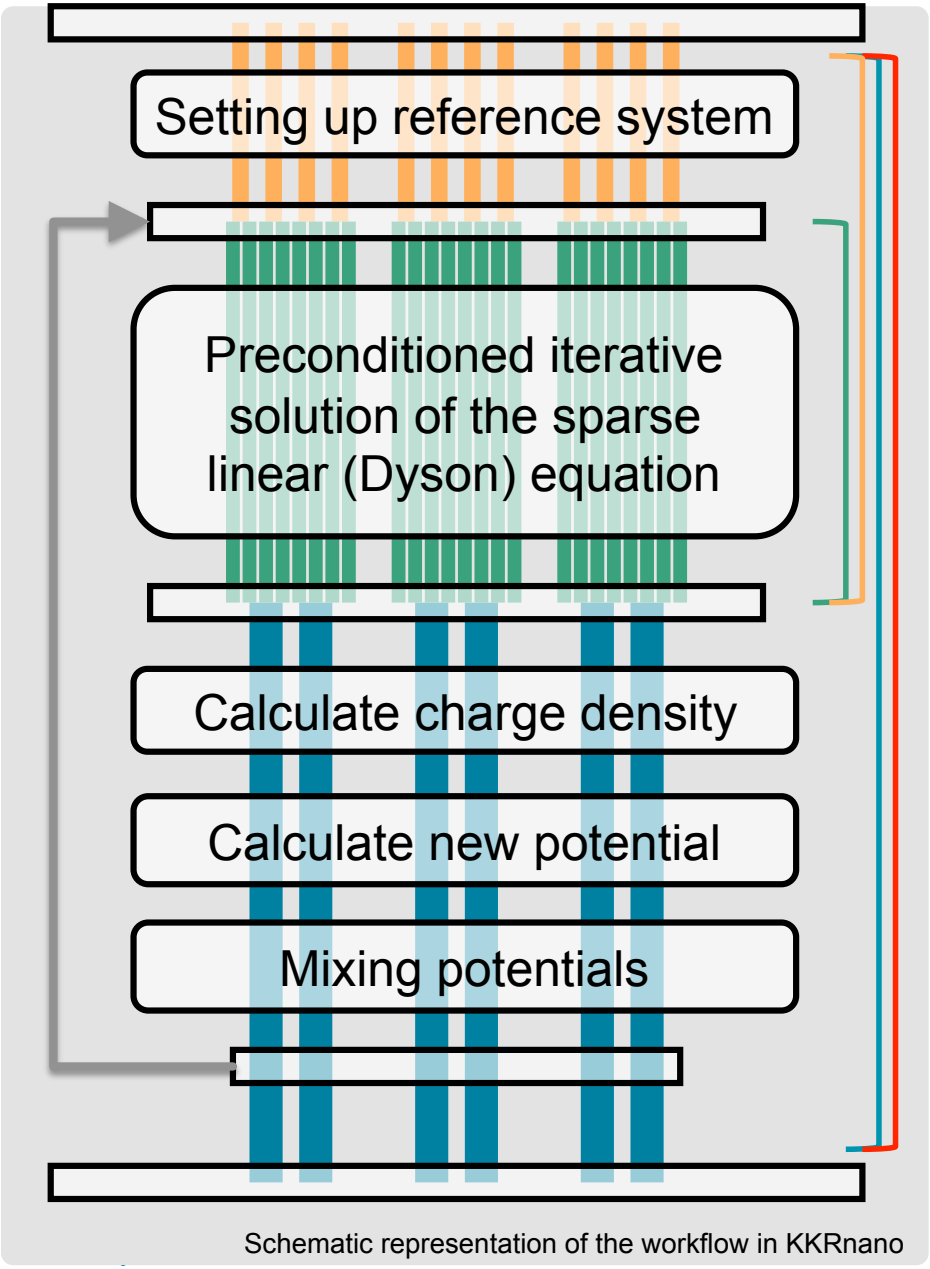
Dyson equation

$$\hat{G} = \hat{G}^{\mathrm{ref}} + \hat{G}^{\mathrm{ref}}\, \Delta\hat{t}\, \hat{G}$$



$G(\mathbf{r}, +$
$G^{nn'}_{LL'}$

Solve the Dyson equation by iterative inversion of a huge sparse matrix for multiple RHSs **A** • x = b



Schematic representation of the workflow in KKRnano

Massive parallelization

Parallel over atoms a
[N_{atoms}] MPI processes
1st level

Parallel over spins
[1-2] MPI processes
2nd level

Parallel over energy points
[1-4] MPI processes
dynamically load-balanced
3rd level

OpenMP parallel over a'
[1-16] threads
4th level

in total up to 128 task*threads/atom
e.g. N_{atoms} = 4,096 up to 524,288 ts

KKRnano: I/O profile

Initial Input

atom information as coordinates $\mathbf{R}_a$ and

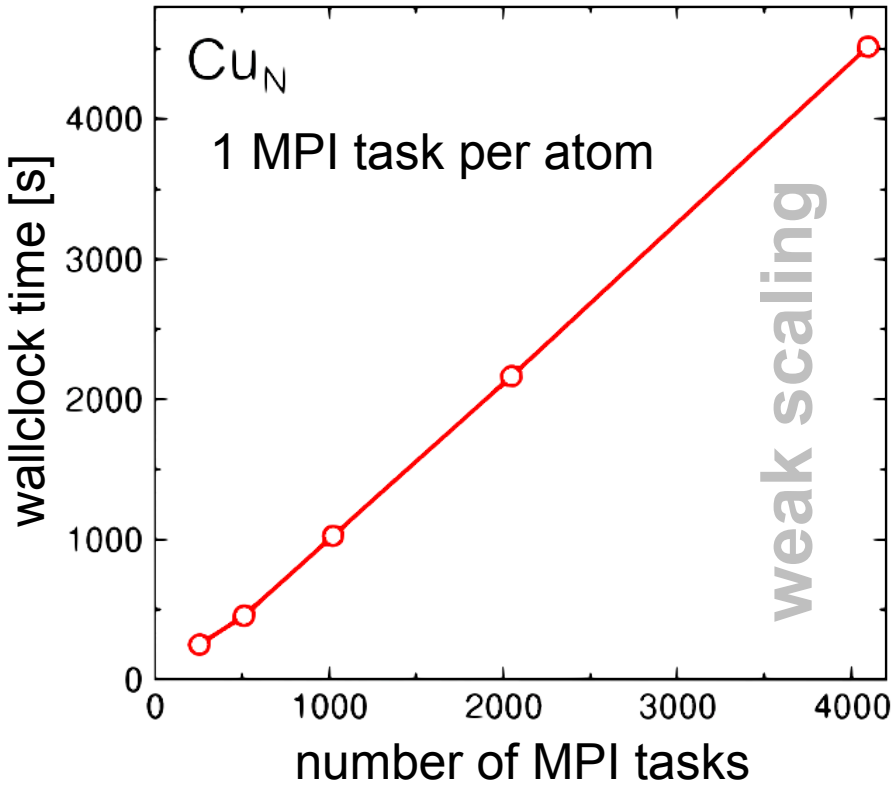
atomic potentials ~640 kByte per atom, DirectAccess file

Log output (ASCII) by master

Final output of the atomic potentials ~640 kByte/atom, DA

No need for Active Storage?

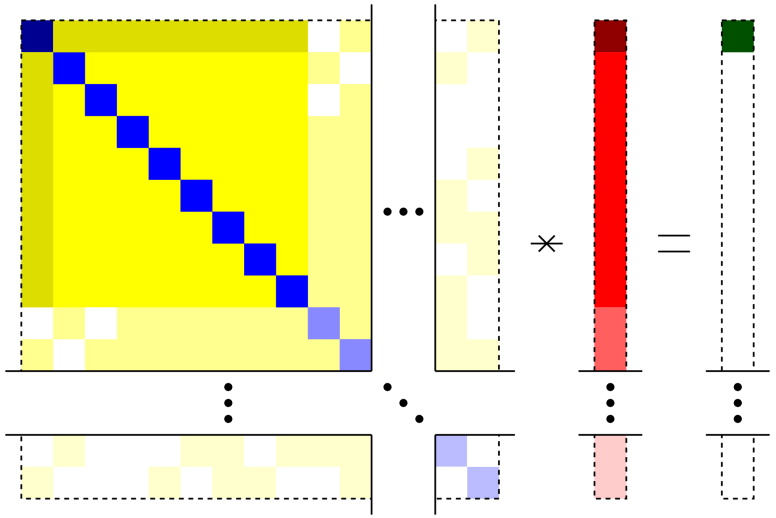
KKRnano: Scaling



CPU-time & Memory ~ N_{atoms}^2 ➔ linear per node

KKRnano: Application of Active Storage

Memory requirement / node linear in N_{atoms} ➔ hard limited by memory
memory prefactor ~ reference cluster range: 1st shell 13, 2nd shell 55

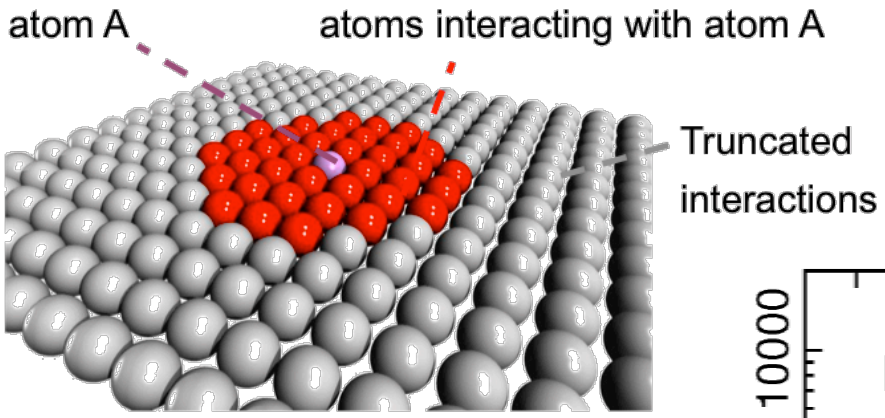


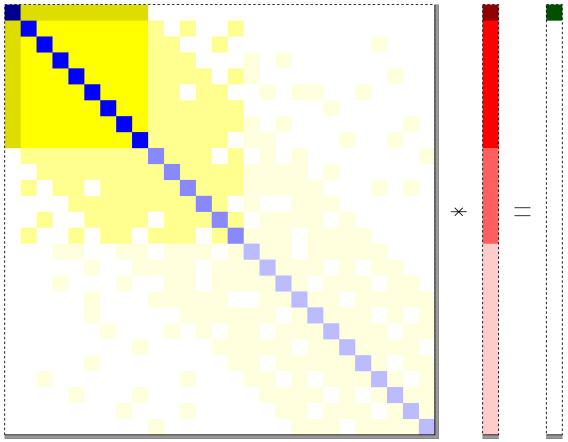
matrix scheme
each atomic block $\in \mathbb{C}^{16\times16}$

Solution of $\mathbb{A} \bullet x = b$ with multiple (16) right hand sides

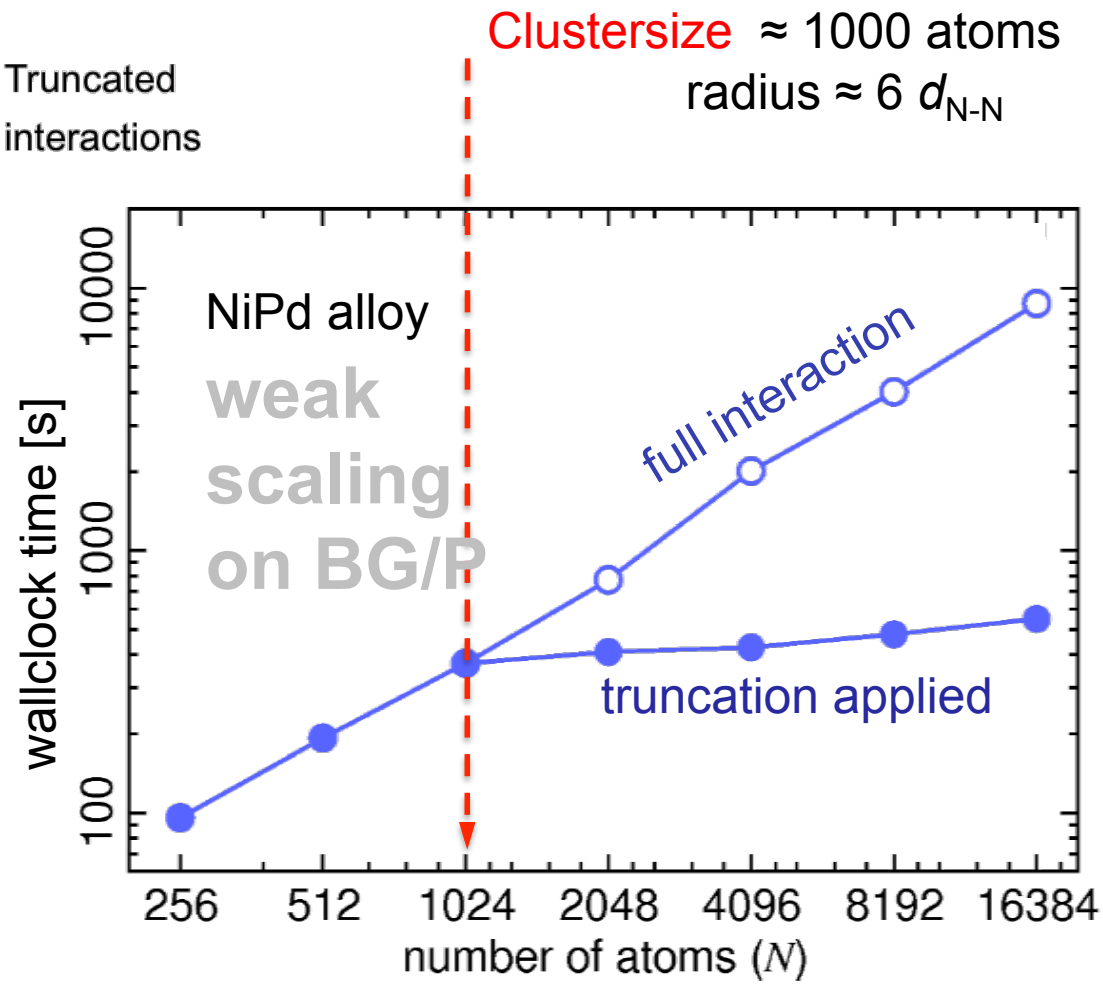
ⓘ use Active Storage to avoid memory issue for matrix elements

KKRnano: Truncation for Linear Scaling





matrix scheme $\mathbf{A} \cdot \underline{x} = \underline{b}$



Summary

Density Functional Theory
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RealSpace juRS
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use AS as local scratch and for checkpointing

MultipleScattering KKRnano
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use AS to extend memory

visit www.ju*DFT*.de

Condensed Matter Codes

Potential Application of Active Storage

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Thank you!