

Real space DFT: SPARC

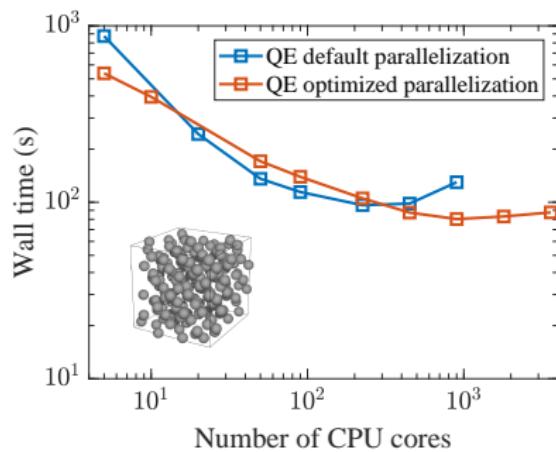
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QM/MM and ab initio Molecular Dynamics Summer School
Institute for Computational Molecular Science Education

Motivation for real-space methods

- Planewave codes (i.e., Fourier basis) among the most widely used in Kohn-Sham DFT, e.g., VASP, Quantum Espresso (QE), ABINIT, ...
- Limitations
 - Artificial periodicity: Isolated systems, crystal defects, electric fields, ...
 - Global nature of basis hampers parallel scalability



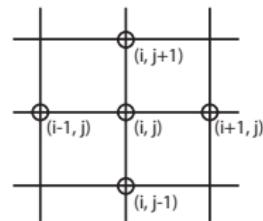
Strong scaling of QE for 216-atom carbon system (Stephen E. Weitzner)

- $\mathcal{O}(N)$ methods?

Real-space DFT

- Real-space discretizations: **Finite-differences**, finite-elements, wavelets, ...
- High-order centered finite-differences for differential operators, e.g.,

$$\nabla_h^2 f|^{(i,j,k)} \approx \sum_{p=0}^{n_o} w_p \left(f^{(i+p,j,k)} + f^{(i-p,j,k)} + f^{(i,j+p,k)} + f^{(i,j-p,k)} \right. \\ \left. + f^{(i,j,k+p)} + f^{(i,j,k-p)} \right)$$



- Integration using the trapezoidal rule:

$$\int_{\Omega} f(\mathbf{x}) d\mathbf{x} \approx h^3 \sum_{i=1}^{n_1} \sum_{j=1}^{n_2} \sum_{k=1}^{n_3} f^{(i,j,k)}$$

- Attractive features

- Standard eigenvalue problem with small spectral width
- Employ and switch between high-order approximations
- Compact representation of Laplacian
- Periodic, non-periodic, and other boundary conditions
- Amenable to scalable high performance computing

SPARC electronic structure code

The screenshot shows the GitHub repository page for `SPARC-X / SPARC`. The repository has 340 commits across 2 branches and 1 tag. Key commits include updates to documentation, pseudopotential files, and testing. The repository is described as a "Simulation Package for Ab-initio Real-space Calculations" with tags for HPC, large-scale, massively-parallel, boundary-conditions, electronic-structure, kohn-sham, aimd, easy-install, finite-difference-method, dft-calculations, structural-optimization, and real-space. It has 32 stars, 8 watchers, 18 forks, and a Readme and GPL-3.0 license. A release v1.0.0 was published on May 13, 2021. There are no packages published yet.

SPARC-X / SPARC Public

Code Issues Pull requests Discussions Actions Projects Wiki Security Insights Settings

master 2 branches 1 tag Go to file Add file Code

phanih-suryanarayana Merge pull request #118 from xugimen/master 8159432 2 hours ago 340 commits

doc Modify funding info in README.md, documentation, and .out files last month

lib first commit 2 years ago

pssps Updated (detailed citation) pseudopotential files 11 days ago

src modify ChangeLog and version date 4 hours ago

tests Update tests 4 days ago

.gitignore bug fixed in stress 5 months ago

.gitmodules first commit 2 years ago

.travis.yml made automatic testing ON 2 years ago

ChangeLog modify ChangeLog and version date 4 hours ago

LICENSE first commit 2 years ago

README.md Update README.md 12 days ago

README.md

SPARC installation and usage

About

Simulation Package for Ab-initio Real-space Calculations

HPC large-scale massively-parallel
boundary-conditions electronic-structure
kohn-sham aimd easy-install
finite-difference-method dft-calculations
structural-optimization real-space

Readme GPL-3.0 license

32 stars 8 watching

18 forks

Releases 1

SPARC v1.0.0 Latest on May 13, 2021

Packages

No packages published Publish your first package

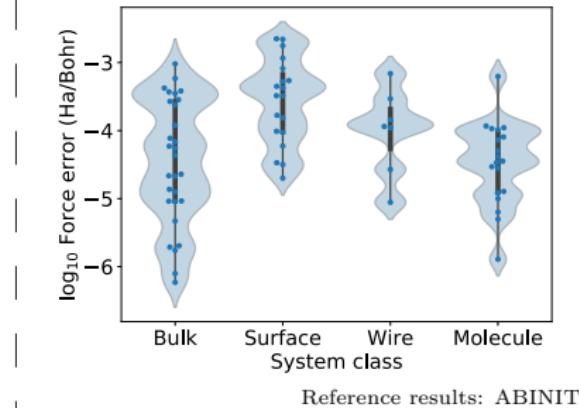
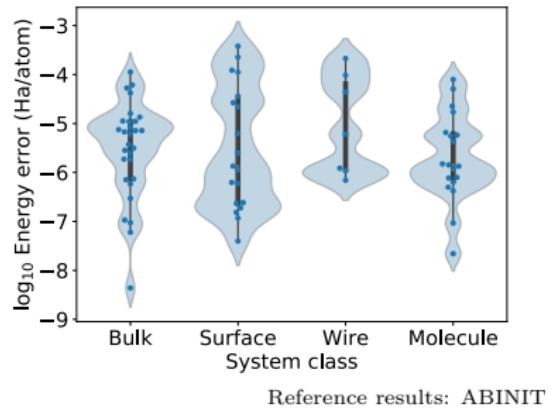
- SPARC is portable and straightforward to install, use, and modify.
- External dependencies limited to industry standard BLAS, LAPACK/ScaLAPACK, and MPI.

SPARC: Features

- Isolated systems such as molecules as well as extended systems such as crystals, surfaces, and wires.
- Local, semilocal, and nonlocal (including hybrid) exchange-correlation functionals.
- Standard ONCV pseudopotentials, including nonlinear core corrections.
- Calculation of ground state energy, atomic forces, and stress tensor.
- Structural relaxation and ab initio molecular dynamics (NVE, NVT, and NPT).
- Spin polarized and unpolarized calculations.
- Spin-orbit coupling.
- Dispersion interactions through DFT-D3, vdW-DF1, and vdW-DF2.
- Orbital-free DFT with TFW, WT, and WGC kinetic energy functionals.
- MATLAB version available for rapid prototyping: M-SPARC.
- Symmetry adaption for cyclic and helical symmetries.
- $\mathcal{O}(N)$ Spectral Quadrature (SQ) method.
- Discrete Discontinuous Basis Projection (DDBP) method
- Density Functional Perturbation Theory (DFPT)
- RPA correlation energy
- On-the-fly machine learned force fields (MLFFs)

SPARC: Accuracy

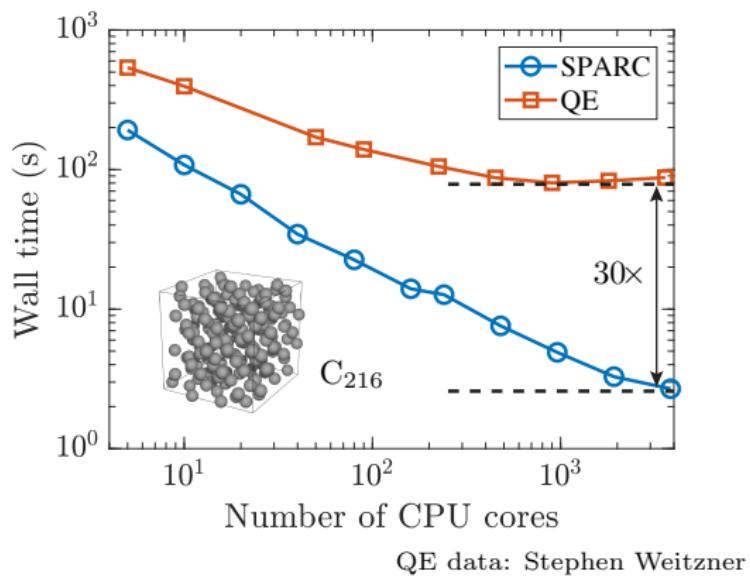
- Accuracy of SPARC has been carefully established. (*Xu et. al., 2021*)



- 74-system test suite
- SPARC: 0.2 bohr, ABINIT: 100 Ha
- Average energy error: 2e-5 Ha/atom
- Average force error: 2e-4 Ha/Bohr
- Agreement improves even further with finer grid

SPARC: Performance

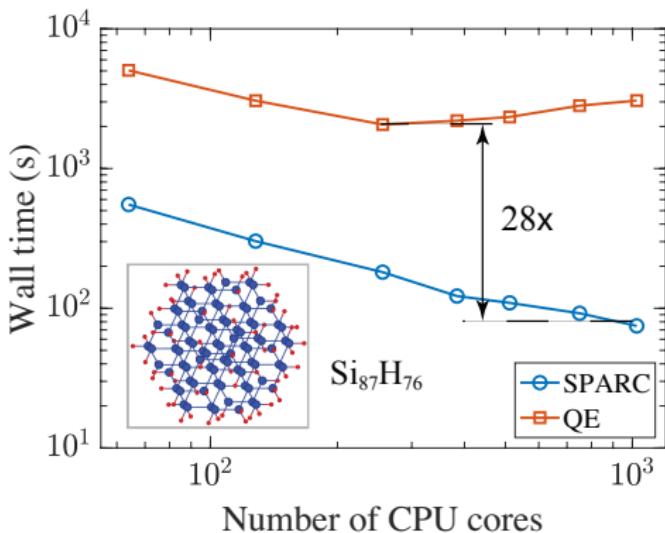
- Exchange-correlation: PBE ($E_{xc}(\rho, \nabla\rho)$) (Xu et. al., 2021)



- More than an order-of-magnitude speedup in time to solution.

SPARC: Performance

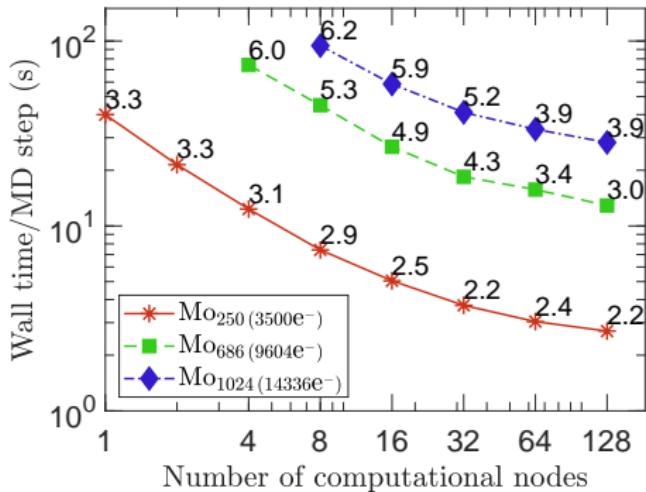
- Exchange-correlation: PBE0 ($E_{xc}(\rho, \nabla\rho, \Psi)$) (Zhang et. al., 2024)



- More than an order-of-magnitude speedup in time to solution.

SPARC: GPU Acceleration

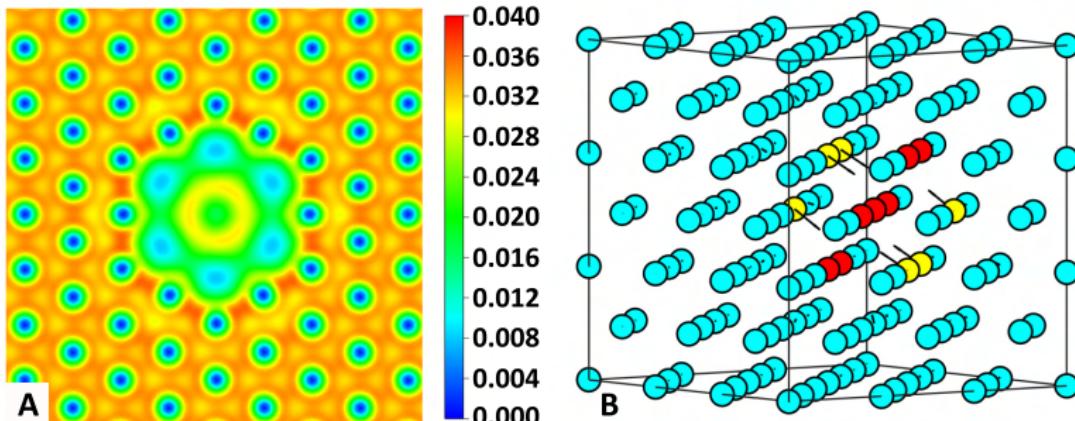
- Modern supercomputers have the option of GPU acceleration.
- Exchange-correlation: PBE ($E_{xc}(\rho, \nabla\rho)$) (Sharma et. al., 2023)



- Lassen supercomputer at LLNL: 4 GPUs and 40 CPUs
- Speedup in core hours a factor of 10 larger

Prismatic dislocation loop in Aluminum

- Studied the collapse of vacancies into a prismatic dislocation loop in Aluminum.
(Bhowmik et. al., 2025)



- >1000 atoms
- 27 k-points
 - Wavevectors obtained upon reduction of supercell to current cell
 - $\psi_n(\mathbf{x} + \mathbf{R}) = e^{i\mathbf{k}\cdot\mathbf{R}}\psi_n(\mathbf{x})$
- 10^{-5} ha/atom accuracy in the energy

Concluding remarks

- SPARC is an accurate, efficient, and scalable open-source electronic structure code.
- Many advanced features, able to efficiently leverage moderate and large-scale computational resources alike.
- Straightforward to install, use, and modify, with minimal external library dependencies.
- An **order of magnitude faster than state-of-the-art planewave codes**, with a range of exchange-correlation functionals, and with increasing advantages as the number of processors is increased.
- SPARC efficiently scales to thousands of processors in regular operation, bringing solution times down to about **a minute for systems with $O(500\text{-}1000)$ atoms**, and **a few seconds for $O(100\text{-}500)$ atoms**.
- GPU acceleration: **diagonalization speedup of 5–12x**. Public release soon.
- **Cyclic+helical symmetry adaption**. Efficient study of nanostructures/nanomaterials and their response to mechanical deformations.
- **$O(N)$ SQ method**, it has been scaled to system sizes of over a **million atoms**.
- **Study of warm dense matter (WDM)**

Acknowledgements

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Thank You!
Questions?