ELSI: A Unified Software Interface for Kohn-Sham Electronic Structure Solvers

Victor Yu and the ELSI team

Department of Mechanical Engineering & Materials Science
Duke University

Kohn-Sham Density-Functional Theory

Atomistix ToolKit

BigDFT

CP2K

DGDFT

DFTB

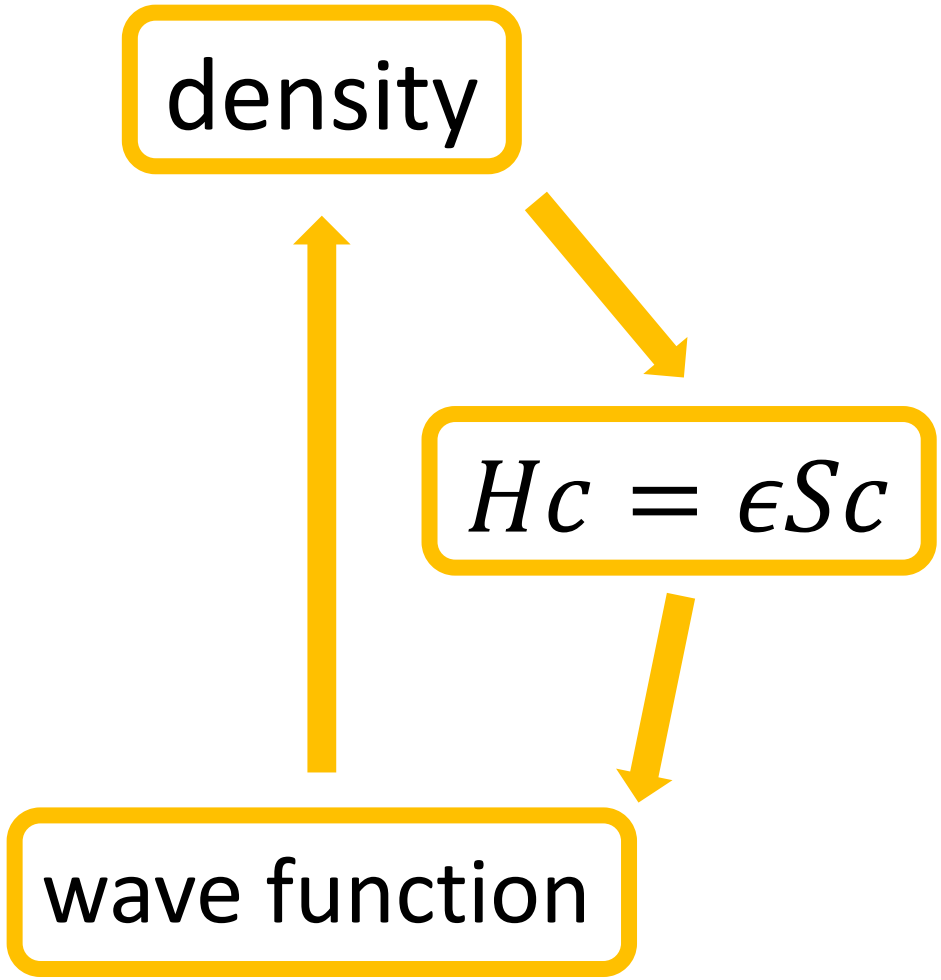
The ab initio molecular simulations package FHI aims

NWChem

QUANTUMESPRESSO

siesta

VASP b-initio ienna ackage imulation



L.M. Ghiringhelli et al., Towards a Common Format for Computational Materials Science Data, Psi-k Scientific Highlight of the Month 131, July 2016.

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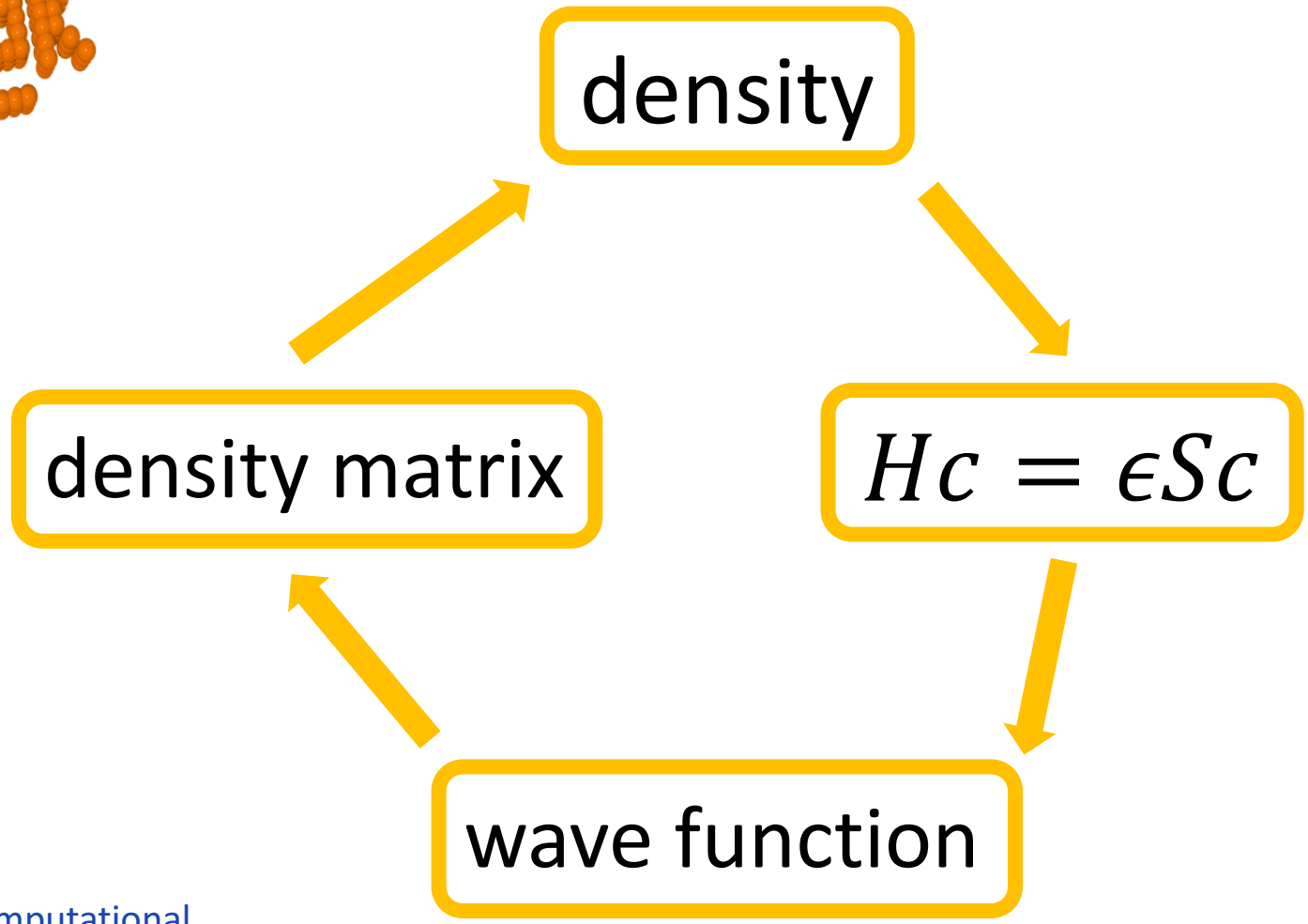

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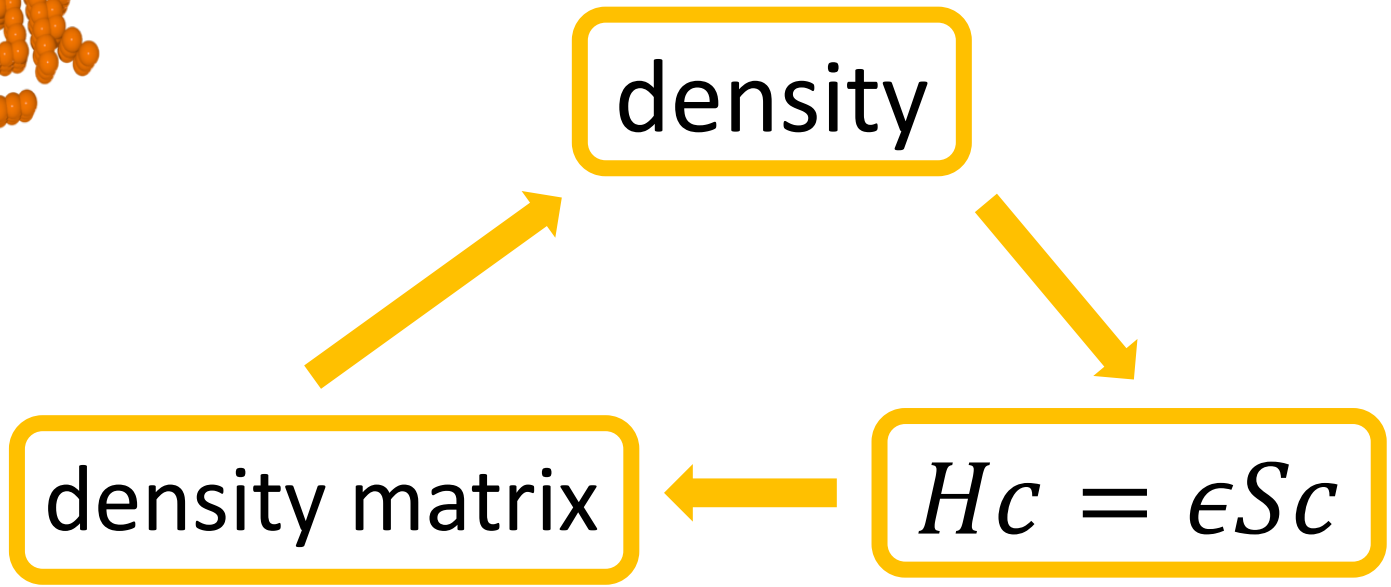

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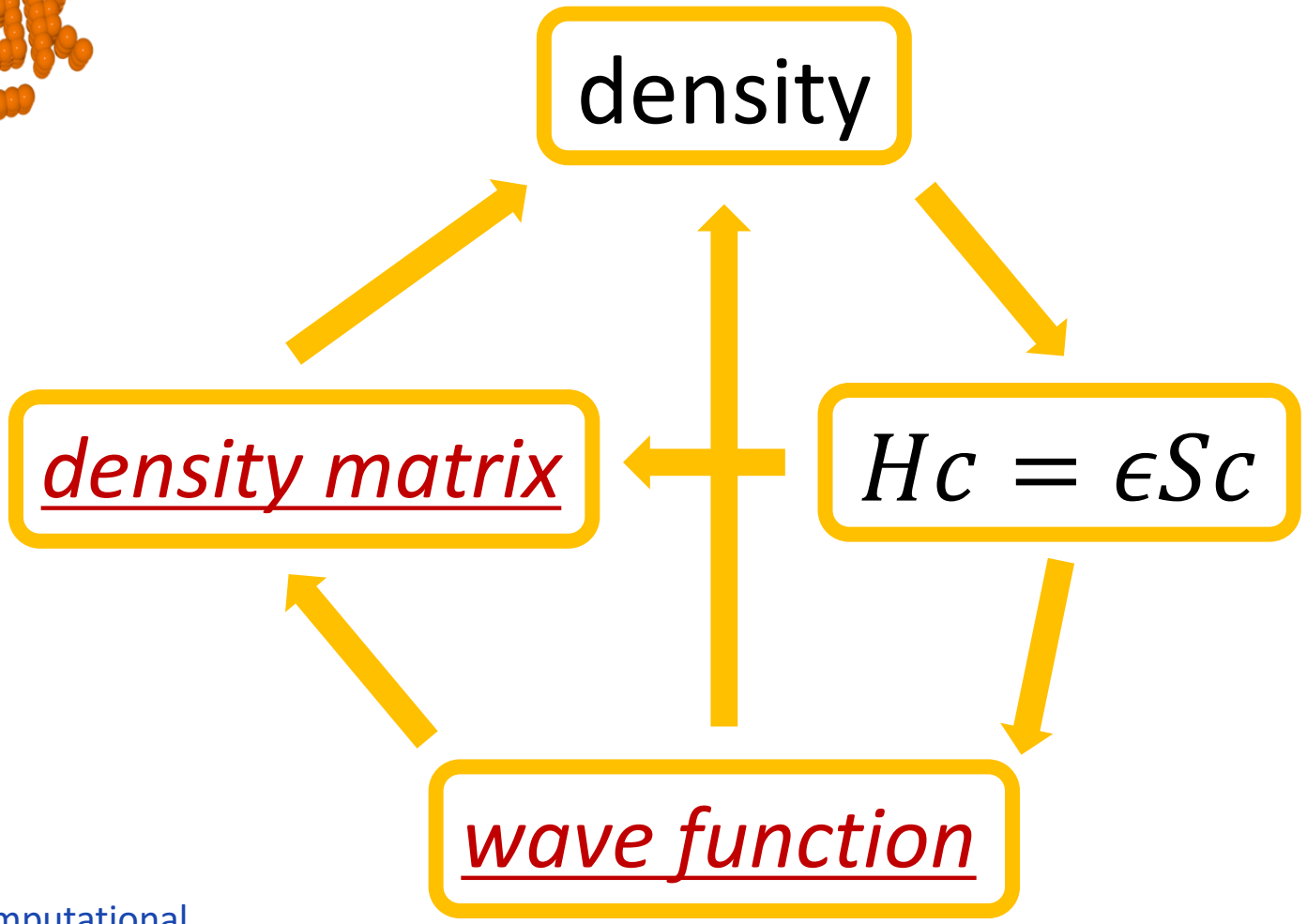
VASP: Vienna Ab-initio Simulation Package



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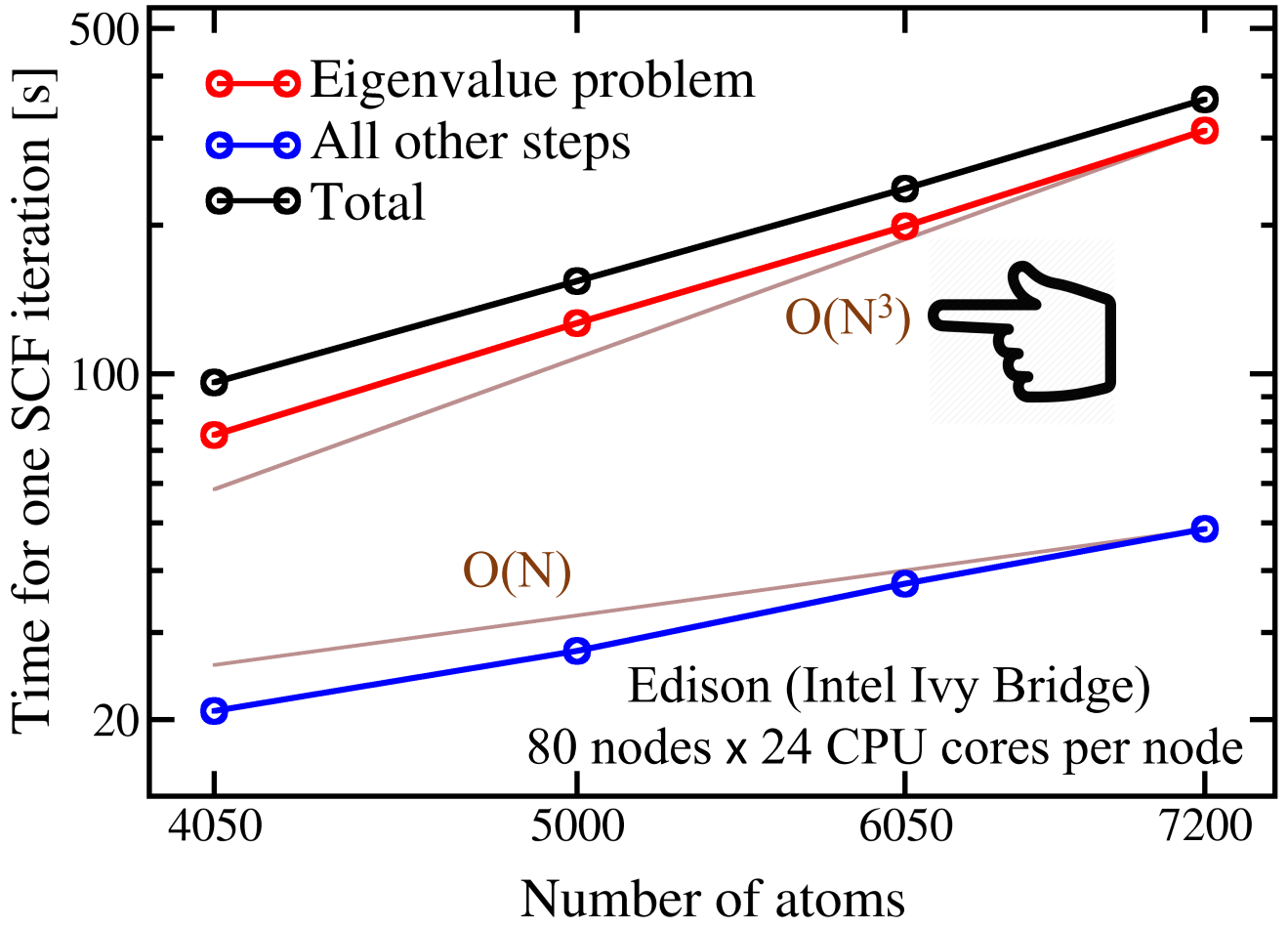
The "Cubic Wall" in Kohn-Sham Density-Functional Theory

- DFT-PBE with FHI-aims
- Graphene monolayer (2D)
- From 4,050 to 7,200 atoms
- 14 numeric atom-centered orbitals per carbon atom

The *O(N³)* Kohn-Sham eigenproblem must be addressed by *all* electronic structure codes based on KS-DFT

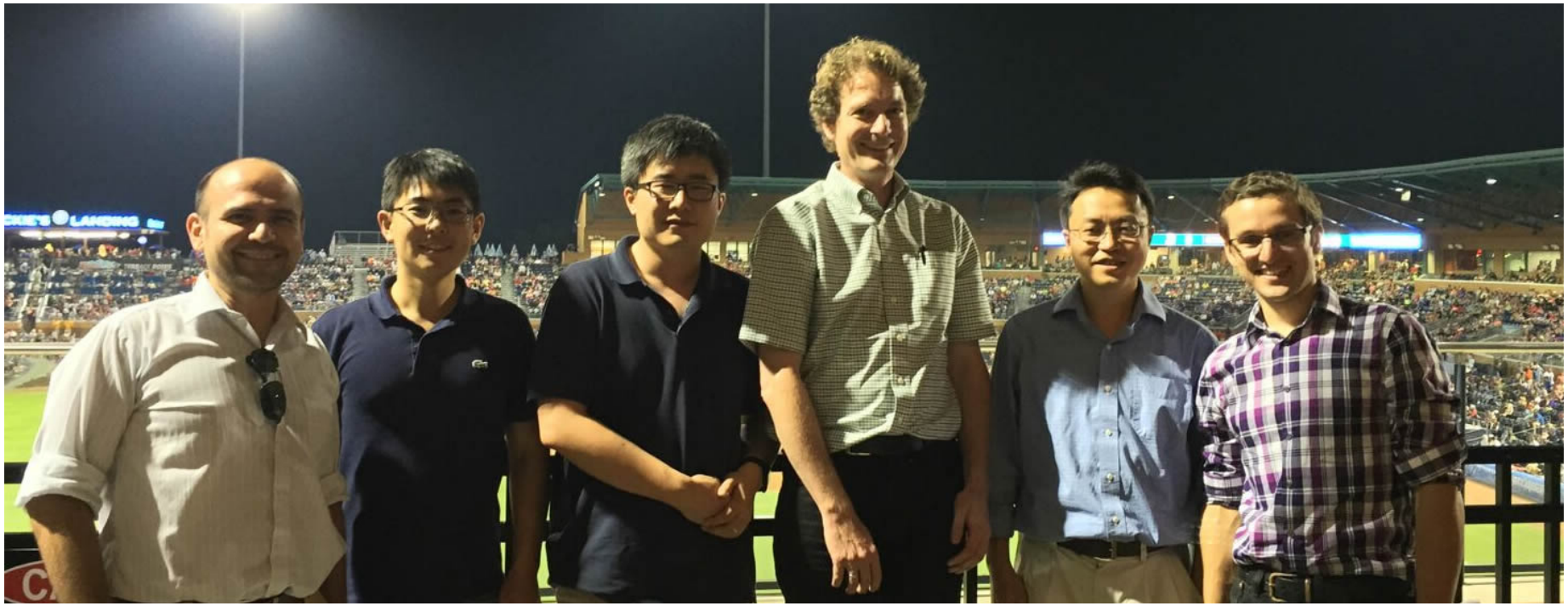


Kohn-Sham Electronic Structure Solvers

ELPA (eigensolution) Dense, direct eigensolver $O(N^3)$	*PEXSI* (density matrix) Pole expansion, selected inversion $\leq O(N^2)$	*CheSS* (density matrix) Chebyshev expansion $O(N)$
libOMM (density matrix) Orbital minimization $O(N^3)$ reduced prefactor	*SIPs* (eigensolution) Sparse, iterative eigensolver $\leq O(N^2)$	And many others, e.g. iterative solvers and ScaLAPACK

A unified software interface
and solver comparison platform

ELSI Timeline



ELSI Kick-Off Meeting, Duke University, Durham, 2017

Aug 2015

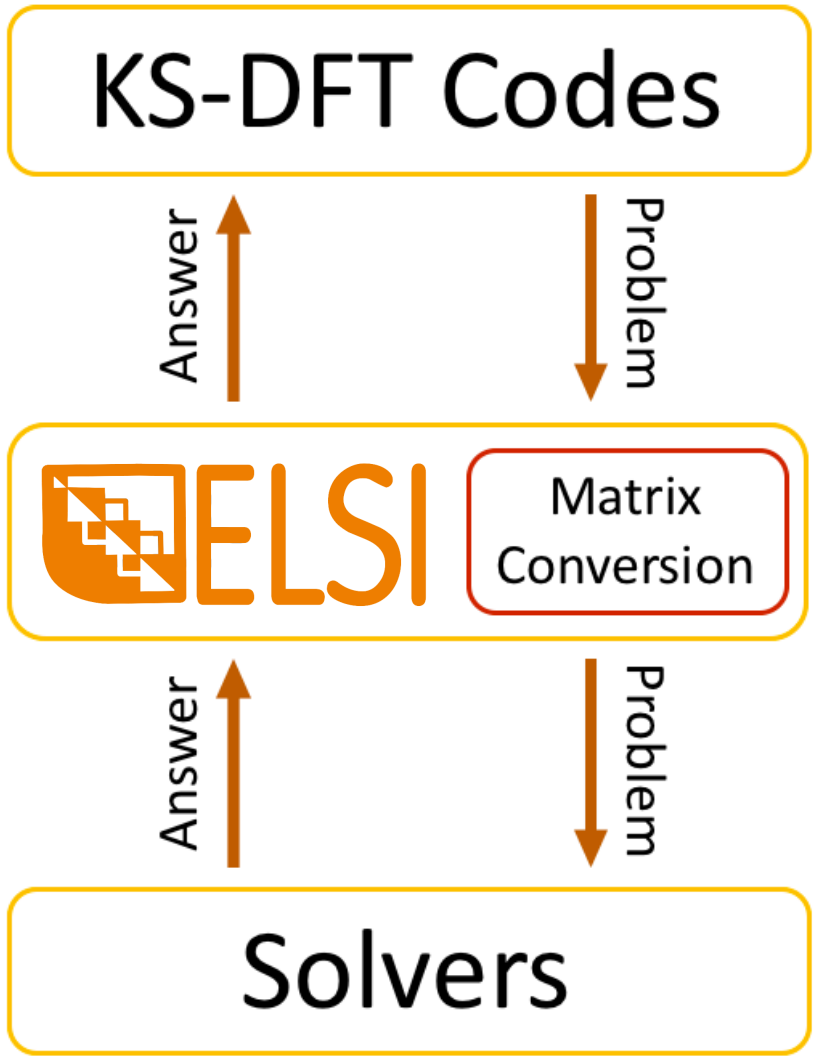
ELSI: Connection between DFT Codes and KS Solvers

KS-DFT Codes ← Create Hamiltonian and overlap matrices

- Different matrix storage strategies
- Different application programming interfaces
- Different programming languages

Solvers ← Compute eigenvalues, eigenvectors, density matrix

ELSI: Connection between DFT Codes and KS Solvers



Create Hamiltonian and overlap matrices

- Convert data format and distribution automatically
- Analyze the problem:
  Basis set size, sparsity, desired output, available computational resource, … (*ongoing*)
- Suggest a solver with reasonable settings (*future*)

Compute eigenvalues, eigenvectors, density matrix

ELSI Timeline

Electronic Structure Library Coding Workshop, ZCAM, Zaragoza, 2016

Aug 2015 Jun 2016

Philosophy of the ELSI Interface

Easy to implement

Designed to be flexible for rapid integration into a variety of KS-DFT codes

Versatile

Includes density matrix and eigensystem formalisms on equal footing

Flexible

All technical settings in solver libraries are adjustable for experienced users

API of ELSI interface

```
elsi_init
! BEGIN SCF LOOP
    elsi_set
    elsi_{dm|ev}
! END SCF LOOP
elsi_finalize
```

ELSI Timeline

First Release of ELSI

Aug 2015 Jun 2016 May 2017

First Release of ELSI: May 2017

http://elsi-interchange.org

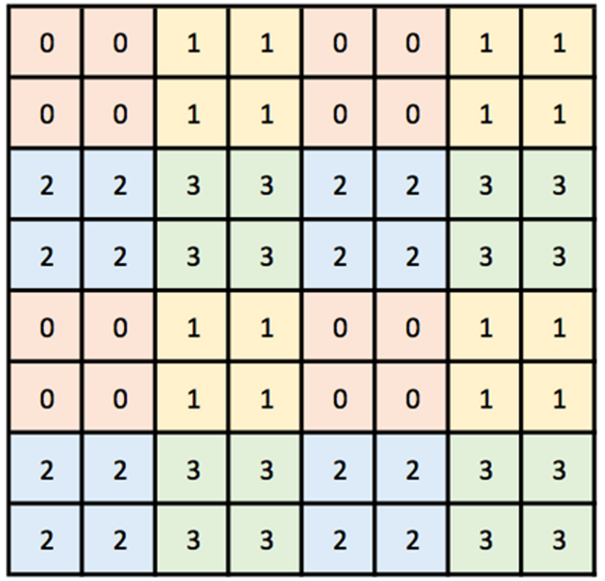
- *Software Package*
  - ELSI interface
  - Current ELPA, libOMM, PEXSI
- *Programming Language*
  - Fortran 2003
  - C/C++ interface
- *Functionalities*
  - Eigenvalues and eigenvectors
  - Density matrix
  - Chemical potential
  - Occupation numbers
- *Portability*
  - GNU, Intel, PGI, IBM, Cray
  - Cori, Edison, Mira, Theta, Titan
- *Flexibility*
  - 2 matrix I/O formats
  - 2 parallel modes
  - Concurrent instances
  - Tested in DGDFT, FHI-aims, NWChem (Global Arrays), SIESTA
- *Scalability*
  - (Hundreds of) thousands of MPI tasks

Supported Matrix Formats

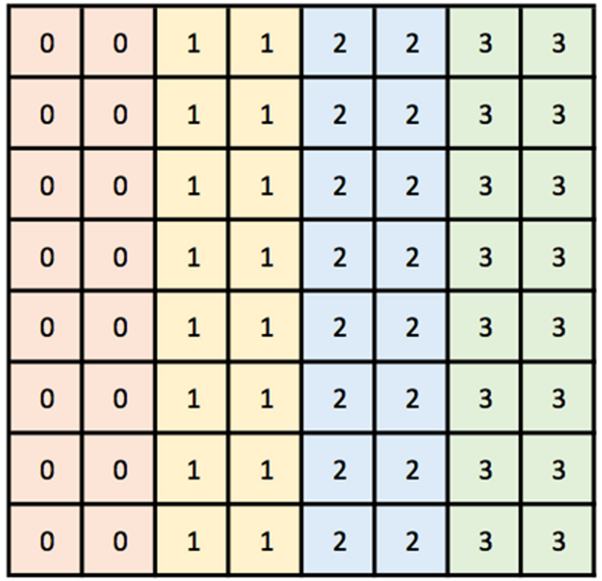
a) 2D block-cyclic distributed dense storage (BLACS standard)

b) 1D block distributed compressed column storage (PEXSI standard)

c) 1D block distributed compressed row storage supported implicitly due to symmetry



(a)



(b)

Auto-conversion between (a) and (b) when necessary

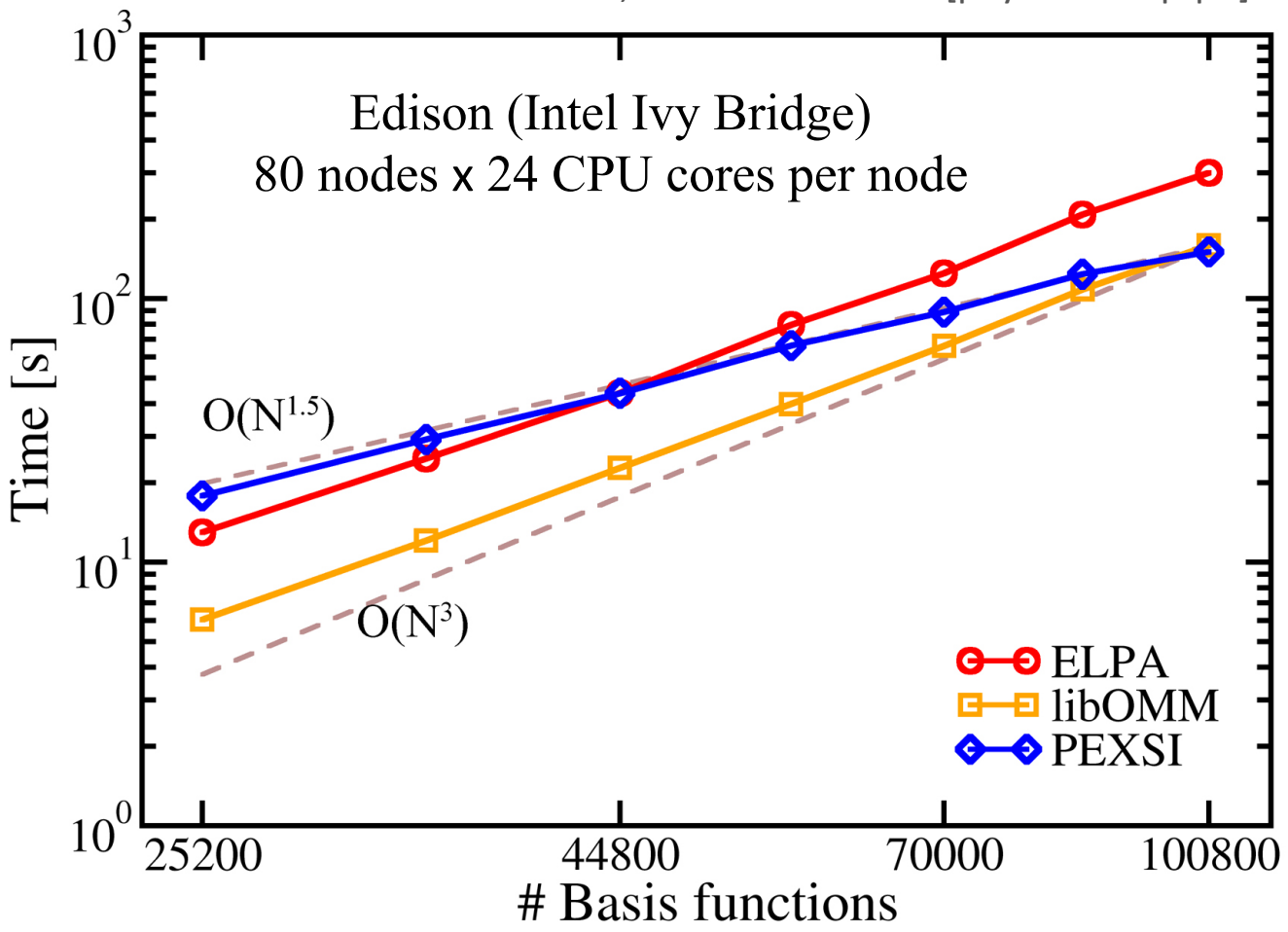
Example: BLACS input ➔ PEXSI format ➔ PEXSI solver ➔ BLACS output

Performance of the Solvers (ELSI May 2017)

- DFT-PBE with FHI-aims
- Graphene monolayer (2D)
- From 1,800 to 7,200 atoms
- 14 numeric atom-centered orbitals per carbon atom

PEXSI starts outperforming ELPA and libOMM at *3,000* and *7,000* atoms, respectively

V. Yu et al., ELSI: A Unified Software Interface for Kohn-Sham Electronic Structure Solvers, arXiv:1705.11191 [physics.comp-ph].

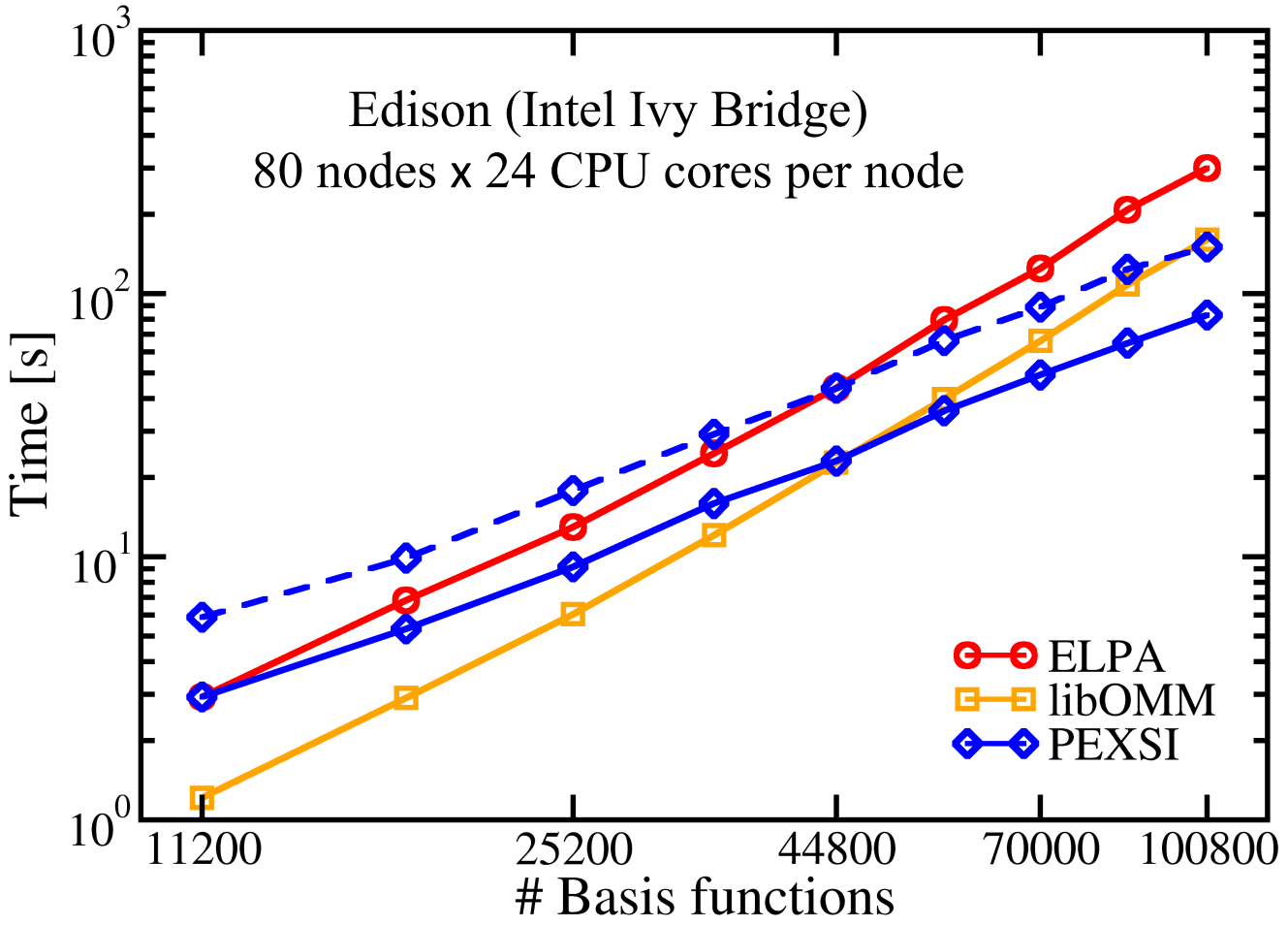


Performance of the Solvers (Today)

- DFT-PBE with FHI-aims
- Graphene monolayer (2D)
- From 800 to 7,200 atoms
- 14 numeric atom-centered orbitals per carbon atom

PEXSI starts outperforming ELPA and libOMM at ~~3,000~~ *800* and ~~7,000~~ *3,200* atoms, respectively!

Up-to-date



Enhanced Feature: Energy-Weighted Density Matrix

	ELPA	libOMM	PEXSI
DM	$C_{DM}C_{DM}^T$	$W(2I_W - S_W)W^T$	$\mathrm{Im}\sum_{l=1}^{P}\frac{w_l^{DM}}{H-(z_l+\mu)S}$
EDM	$C_{EDM}C_{EDM}^T$	$W[(2I_W - S_W)H_W]W^T$	$\mathrm{Im}\sum_{l=1}^{P}\frac{w_l^{EDM}}{H-(z_l+\mu)S}$

- Pulay force (localized orbitals)
- Available with all three solvers
- Only computed when calling *elsi_get_edm*

✓ Geometry optimization

ELSI Timeline

Electronic Structure Library Coding Workshop, ICTP, Trieste, 2017

Aug 2015 Jun 2016 May 2017 Jul 2017

Enhanced Feature: K-Point and Spin Calculations

New MPI communicator for communications among all k-points and spins

```
elsi_init(handle,...)

! Set MPI communicator
elsi_set_mpi(handle,my_mpi_comm)
elsi_set_mpi_all(handle,mpi_comm_all)

! Set spin and/or k-point
elsi_set_spin(handle,n_spin,my_spin)
elsi_set_kpt(handle,n_kpt,my_kpt,my_weight)

! Compute density matrices
elsi_dm_real(handle,my_H,my_S,my_DM,energy)

elsi_finalize(handle)
```

Enhanced Feature: K-Point and Spin Calculations

New Number of spins and my spin index

```
elsi_init(handle,...)

! Set MPI communicator
elsi_set_mpi(handle,my_mpi_comm)
elsi_set_mpi_all(handle,mpi_comm_all)

! Set spin and/or k-point
elsi_set_spin(handle,n_spin,my_spin)
elsi_set_kpt(handle,n_kpt,my_kpt,my_weight)

! Compute density matrices
elsi_dm_real(handle,my_H,my_S,my_DM,energy)

elsi_finalize(handle)
```

Enhanced Feature: K-Point and Spin Calculations

New Number of k-points, my k-point index, and my k-point weight

```
elsi_init(handle,...)

! Set MPI communicator
elsi_set_mpi(handle,my_mpi_comm)
elsi_set_mpi_all(handle,mpi_comm_all)

! Set spin and/or k-point
elsi_set_spin(handle,n_spin,my_spin)
elsi_set_kpt(handle,n_kpt,my_kpt,my_weight)

! Compute density matrices
elsi_dm_real(handle,my_H,my_S,my_DM,energy)

elsi_finalize(handle)
```

Enhanced Feature: K-Point and Spin Calculations

- Minimal additions to the existing ELSI interface
- Capability to handle k-point and/or spin in parallel
- No overhead if not interested in k-point and/or spin

✓ Spin ✓ K-point

```
elsi_init(handle,...)

! Set MPI communicator
elsi_set_mpi(handle,my_mpi_comm)
elsi_set_mpi_all(handle,mpi_comm_all)

! Set spin and/or k-point
elsi_set_spin(handle,n_spin,my_spin)
elsi_set_kpt(handle,n_kpt,my_kpt,my_weight)

! Compute density matrices
elsi_dm_real(handle,my_H,my_S,my_DM,energy)

elsi_finalize(handle)
```

New Feature: CheSS and SIPs Solvers

CheSS (density matrix)

Fermi operator expansion with Chebyshev polynomials

O(N)

SIPs (eigensolution)

Sparse, iterative eigensolver based on spectrum slicing

$\leq O(N^2)$

- Both solvers connected to ELSI
  - SOLVER = 4 (CheSS)
  - SOLVER = 5 (SIPs)
- Flexibility of the ELSI infrastructure: Given compatible matrix formats, a new solver can be quickly added to ELSI in hours
- Both are giving correct results
- Todo
  - Performance optimization
  - Benchmark

✓ O(N) solver

✓ Spectrum slicing

ELSI Timeline

Aug 2015 Jun 2016 May 2017 Jul 2017 Future…

Future Plans & Acknowledgments

- Performance-optimized, up-to-date solver libraries
- More matrix formats used in KS-DFT codes to be supported
- Iterative solvers, e.g. Davidson and CG solvers from Quantum Espresso
- Integration of ELSI into KS-DFT codes for production-level usage
- ELSI decision layer for automatic, optimal choice of solvers
- ELSI workshop in 2018

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