Sakurai-Sugiura algorithm based eigenvalue solver for Siesta

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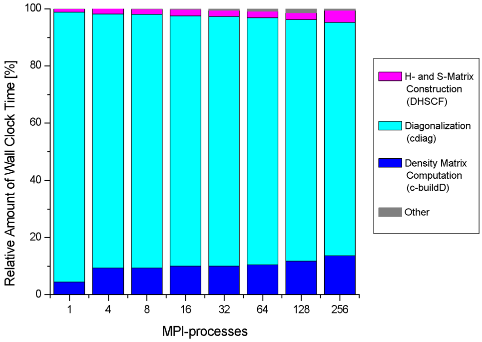
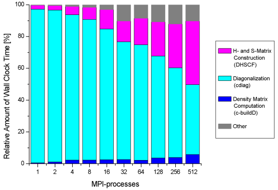
Motivation

Timing analysis for one SCF-loop iteration:





left: CNT/Graphene, right: DNA

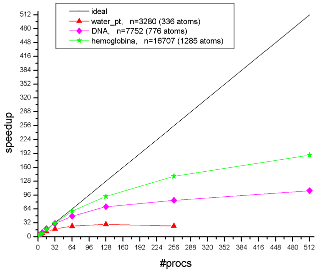
Siesta

Specifics

- High fraction of EVs needed (e.g. 30%)
- Sparse matrices

Actual solver: ScaLAPACK

- Dense solver
- Limited scaling



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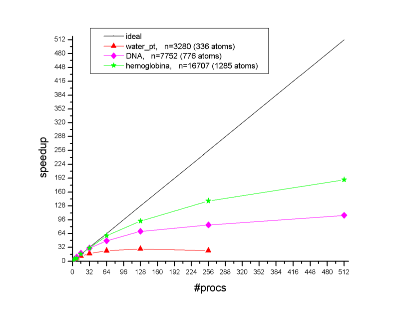


Characteristics

SS-method, Tetsuya Sakurai and Hiroshi Sugiura, 2002

- Solver for GEV $A\,\mathbf{x} = \lambda\,B\,\mathbf{x}$
  $A, B \in \mathbb{C}^{n \times n}$
- Projection method, based on complex contour integration
- Meant for finding EVs in a certain domain
- Suitable for
  - large, sparse matrices
  - parallelisation

Basic steps

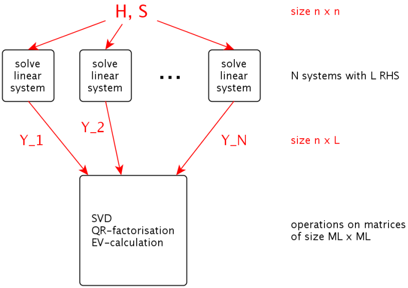
Divide domain of interest into subdomains, in each:

1. Solve a set of linear systems
2. Use results for numerical integrations
3. Construct subspace
4. Find eigenvalues/-vectors in subspace and backtransform
5. Select correct eigenpairs

Parallelisation

Three levels of parallelisation

1. Handling subdomains in parallel
2. Solving N linear systems in parallel
3. Use parallel solver for each linear system



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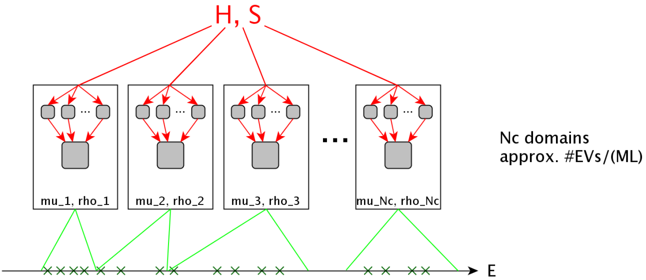

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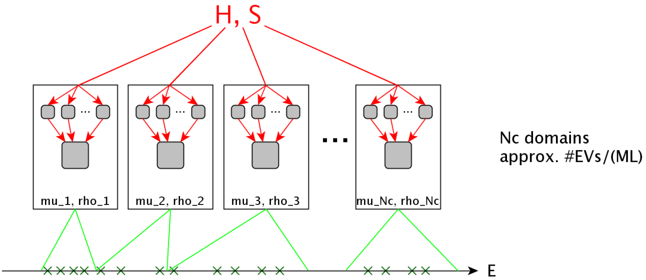
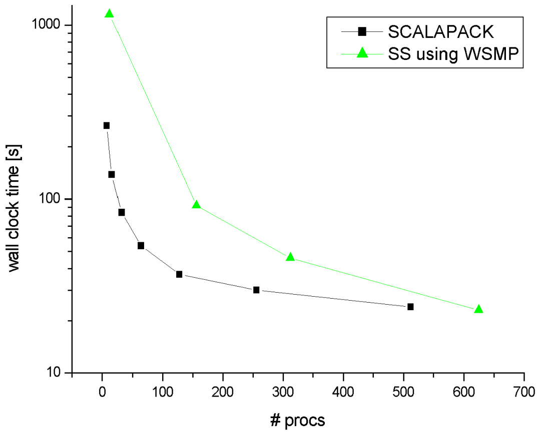


Timing expectations

Example: DNA, 776 atoms, $n = 7752$



Using GPUs

Implemented: Solving the linear systems with CUSP.

Algorithm: gmres without preconditioner!

Gain: Speedup of 3-4 compared to WSMP (for the smaller examples)

Timing solving all lin. systems in parallel (per subdomain)

Problem	Setup	Solve	Comm	total	ScaLAPACK
water_pt ($n = 3280$)	4.0	3.7	0.1	11	7
DNA ($n = 7752$)	3.3	7.6	0.5	13	∼20
hemoglobina ($n = 16707$)	8.0	10	1.0	**22**	**∼70**

All times in seconds

Conclusions

Issues

- Inefficient in serial mode
- Memory parallelisation only in linear solver

Benefits

- Robust algorithm, parameterisation can be hidden from user
- **Actual problems:** SS can be faster than ScaLAPACK, depending on scaling of lin. solver
- **Future problems:** high potential for larger numbers of processors
- Possibility to use many GPUs efficiently

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Thanks to

Alberto García, Pablo Ordejón (Siesta)
Tetsuya Sakurai (Algorithm)
Anshul Gupta (WSMP)

BSC support team
José María Cela (BSC)

More details (1)

1. Define EV-range $\Rightarrow \gamma, \rho$ and a set of vectors $V \in \mathbb{C}^{n \times L}$.
2. Set quatrature points:

$$z_j = \gamma + \rho e^{\left(2\pi \mathrm{i}\left(j+\frac{1}{2}\right)\frac{1}{N}\right)}, \qquad j = 0, \ldots, N-1$$

3. Solve the linear systems

$$(z_j B - A)\, Y_j = B\, V$$

   - N systems, L right hand sides each
   - independent!

More details (2)

4 Numerical integration

$$S_k = \frac{1}{N} \sum_{j=0}^{N/2-1} \left(\frac{z_j - \gamma}{\rho} \right)^{k+1} Y_j, \quad k = 0, \ldots, M-1$$

Matrix $S = [S_0, S_1, \ldots, S_{M-1}] \quad \in \mathbb{C}^{n \times ML}$

5 Find the rank K of S with an SVD and shrink it to $n \times K$

6 QR-decomposition of $S \Rightarrow$ orthogonal basis Q

7 $\tilde{A} = Q^T (A - \gamma B)\, Q$
$\tilde{B} = Q^T B\, Q$ $\qquad \tilde{A}, \tilde{B} \in \mathbb{C}^{K \times K}$

8 Eigenpairs of $\tilde{A}\tilde{\mathbf{x}} = \tilde{\lambda}\tilde{B}\tilde{\mathbf{x}}$

More details (3)

8. Eigenpairs of $\tilde{A}\tilde{\mathbf{x}} = \tilde{\lambda}\tilde{B}\tilde{\mathbf{x}}$
9. Eigenpairs of the original problem

$$\lambda_j = \tilde{\lambda}_j + \gamma$$
$$\mathbf{x}_j = Q \cdot \tilde{\mathbf{x}}_j$$

10. Remove exterior eigenvalues and ghosts.