A 3D-Parallel Interior Eigenvalue Solver

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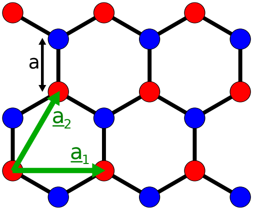
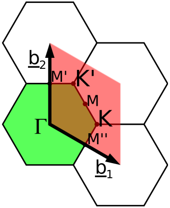
Outline

Graphene Simulation

Graphene



Physical space: carbon atoms in 2D hexagonal mesh

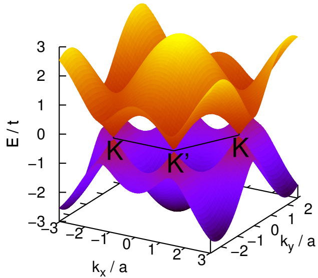


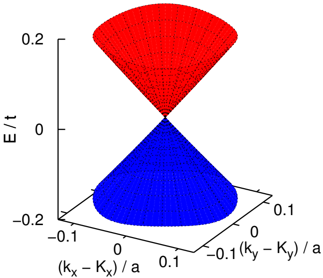
Fourier space ('reciprocal mesh')

Tight-binding Hamiltonian

$$H = \sum_i V_i c_i^\dagger c_i - t \sum_{\langle ij \rangle} (c_i^\dagger c_j + c_j^\dagger c_i)$$

Graphene (2)





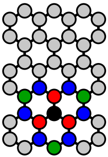
- Analytical solution for infinite Graphene sheet
- Dirac cones: graphene between conductor and semi-conductor

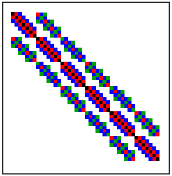
Graphene modeling

- disorder
- long range stencil
- bi-layer
- gate-defined quantum dots
- spin-orbit coupling
- ...

Long range Hamiltonian:

$$H = \sum_i V_i c_i^\dagger c_i - t \sum_{\langle ij \rangle} (c_i^\dagger c_j + c_j^\dagger c_i) - t' \sum_{\langle\langle ij \rangle\rangle} (c_i^\dagger c_j + c_j^\dagger c_i) - t'' \sum_{\langle\langle\langle ij \rangle\rangle\rangle} (c_i^\dagger c_j + c_j^\dagger c_i)$$

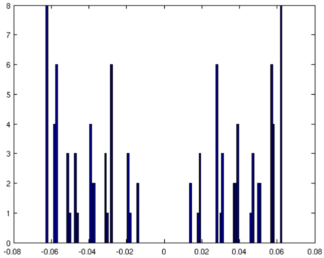




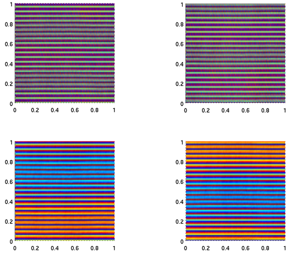
The FEAST Eigensolver

Graphene: eigenmodes of interest

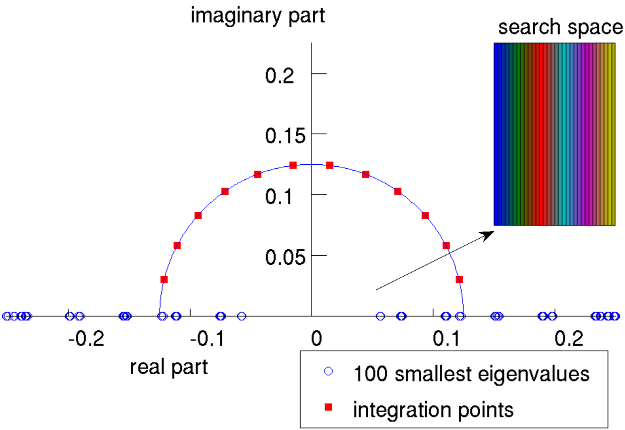
- need many eigenvalues, $\mathcal{O}(1000)$
- in the interior of the spectrum
- tight clusters



- eigenvalue density increases $\sim L$ for $L \times L$ graphene sheet
- rich spectrum of non-smooth modes



FEAST eigensolver (Polizzi '09)



FEAST algorithm for $AX = BX\Lambda$ (A, B symmetric)

Input: $I_\lambda := [\underline{\lambda}, \overline{\lambda}]$, an estimate $\widetilde{m}$ of the number of eigenvalues in I_λ.
Output $\hat{m} \leq \widetilde{m}$ eigenpairs with eigenvalue in I_λ.
Perform:

1. Choose $Y \in \mathbb{C}^{n \times \widetilde{m}}$ of full rank and compute
$$U := \frac{1}{2\pi\mathbf{i}} \int_{\mathcal{C}} (zB - A)^{-1} B \mathrm{d}z \, Y,$$
2. Form $A_U := U^\star A U$, $B_U := U^\star B U$,
3. Solve size-$\widetilde{m}$ eigenproblem $A_U \widetilde{W} = B_U \widetilde{W} \widetilde{\Lambda}$,
4. Compute $(\widetilde{\Lambda}, \widetilde{X} := U \cdot \widetilde{W})$,
5. If no convergence: go to Step 1 with $Y := \widetilde{X}$.

Parallelization of FEAST

Several levels:

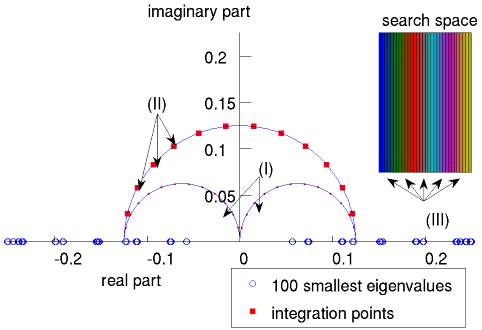
I interval sectioning

II distribute shifts

III distribute right-hand sides

IV parallel linear solver (MPI+X)

V based on SIMD optimized kernels (spMVM, BLAS etc)



Linear Solver: CGMN

Linear systems for FEAST/graphene

Tough:

- very large ($N = 10^8 - 10^{14}$)
- complex symmetric and completely indefinite
- random numbers on and around the diagonal
- spectrum essentially continuous
- shifts get very close to the spectrum

But also nice in some ways:

- 2D mesh, very sparse ($\sim$ 10 entries/row)
- many RHS/shift (block methods, recycling, ...)

An ancient row projection method

- Björck and Elfving, 1979
- CG on the 'minimum norm' problem, $AA^T x = b$
- preconditioned by SSOR
- efficient row-wise formulation
- extremely robust: A may be singular, non-square etc.
- row scaling alleviates issue of 'squared condition number'

Kernel operation: KACZ sweep

Interpretations:

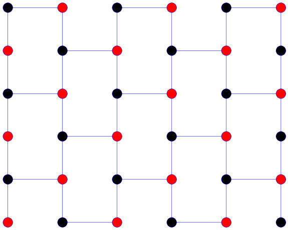
- Kaczmarz algorithm
- SOR(ω) on the normal equations $AA^T x = b$
- successive projections onto the hyperplanes defined by the rows of A

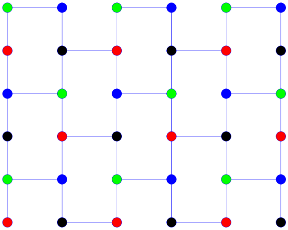
In CRS (rptr,val,col):

```
compute nrms=||a_{i,:}||_2^2
for (i=0; i<n; i++) do
  // compute a_{i,:}x - b_i
    scal=-b[i]
    for (j=rptr[i]; j<rptr[i+1]; j++) do
        scal+=val[j]*x[col[j]]
    end for
    scal/=nrms[i]
  // update x
    for (j=rptr[i]; j<rptr[i+1]; j++) do
        x[cols[j]]-=omega*scal*val[j]
    end for
end for
```

Parallel CGMN

Multi-Coloring (MC) for CGMN





- requires "distance 2" coloring
- software: ColPack
  http://cscapes.cs.purdue.edu/coloringpage/software.htm

Component-Averaged Row Projection (CARP)

- Gordon & Gordon, 2005
- Kaczmarz locally
- write to halo
- exchange and average

Equivalent to Kaczmarz on a superspace of $\mathbb{R}^n$

Hybrid method: MC_CARP-CG

- global MC would require...
  - an extremely scalable coloring method
  - very well-balanced colors
  - many global sync-points ($>$ 20 colors in our examples)
- global CARP would require...
  - huge number of MPI procs
  - increasing amount of 'interior halo elements'
  - non-trivial implementation on GPU and Xeon Phi
  - increasing number of iterations

Idea: node-local MC with MPI-based CARP between the nodes

Experiments

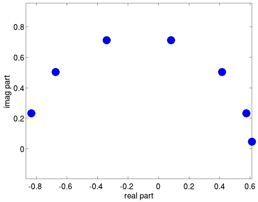
Experimental setup

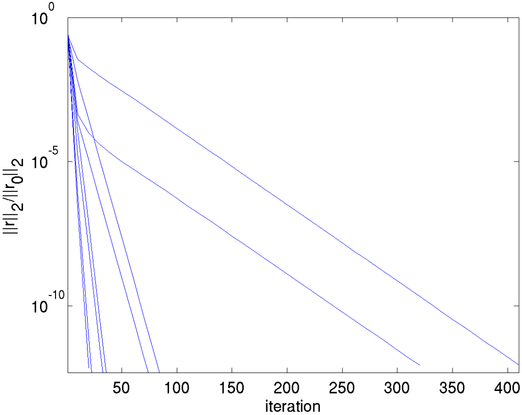
- Machine: Intel Xeon “Ivy Bridge”
- 10 cores/socket, 2 sockets/node
- InfiniBand between nodes

Here's what we do:

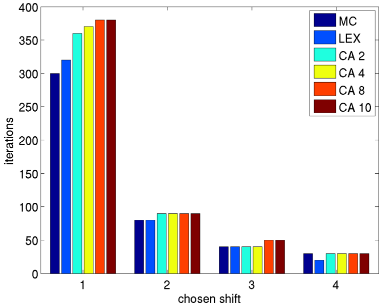
- pick some shifts that may occur in FEAST
- handle 8 RHS at once (for good performance)
- conv tol 10^{-12}
- solve linear systems using CGMN variants

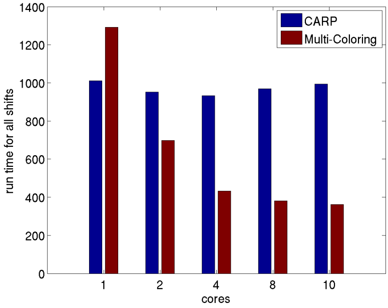
Sequential CGMN for various shifts





Coloring vs. CARP: single socket (1024^2 dof)





Scaling of Hybrid vs. CARP

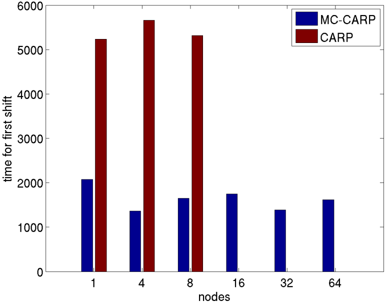


Figure : Weak scaling for Graphene, 4096^2 unknowns per node

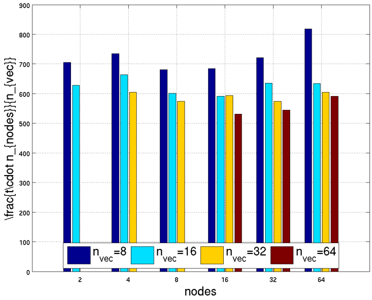
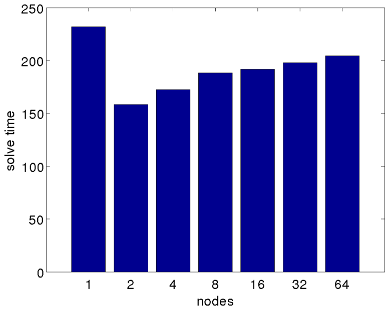


Figure : Strong scaling and block speed-up, 8192^2 unknowns in total

Weak scaling for a 3D benchmark

Synthetic 3D Model of Anderson localization

- uniform 3D grid
- 9-point stencil
- random numbers between -l/2 and l/2 on the diagonal (l=16.5 here)



Summary and Outlook

The (almost) final slide

- Graphene gives nice and challenging test cases for Lin. Alg.
- FEAST requires fast linear solvers for indef. systems
- row projection methods provide the necessary robustness
- algorithm that *calls for* MPI+X parallelization

Future work:

- node-level optimization, GPU and Xeon Phi
- other applications of CGMN: Helmholtz, conv. dom. flow,...
- Multigrid to resolve near kernel problem (?) (cf. recent work by I. Livshits)

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References

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