Truly Scalable $O(N)$ Approach for First-Principles Molecular Dynamics of Non-Metallic Systems

Jean-Luc Fattebert and Daniel Osei-Kuffuor
Center for Applied Scientific Computing
We want to take advantage of growing computational power to simulate larger and more realistic problems in material sciences.

Sequoia, IBM BGQ, 1,572,864 cores

- DFT with Planewaves pseudopotential accuracy (LDA, PBE)
- Fast time to solution
  - 1 step in minutes (not hours!!!) to be useful for MD

Large problems > 5,000 atoms

For insulators, semiconductors

O(N) scalable algorithm
Developing an $O(N)$ algorithm for FPMD implies truncations / approximations

- Unlike classical physics models, in Quantum models the number of physical variables (electrons) grows with system size
  - $\rightarrow O(N^2)$ degrees of freedom and $O(N^3)$ operations in DFT

- Reducing computational complexity to $O(N)$ typically implies
  - Introduction of controllable approximations / truncate fast decaying terms
  - More complicated data structures – sparse vs. full matrices
For systems with band-gap, one can find a representation of the electronic structure with localized functions

- Example: $\text{C}_2\text{H}_4$

- (orthogonal) Maximally Localized Wannier functions
  - Minimize the sum of the spread of all the functions
    - $\sum_{i=1}^{N} \left| \phi_i \right| \left( \hat{X} - \left< \phi_i \middle| \hat{X} \middle| \phi_i \right> \right)^2 \left| \phi_i \right>$
    - [Marzari and Vanderbilt, PRB 1997]

Strictly localized, non-orthogonal, Not centered on atoms (adaptive)

Auxilliary “basis set”
Density Functional Theory: general formulation for non-orthogonal orbitals

- Energy minimization for general non-orthogonal orbitals [Galli and Parrinello, PRL 1992]

\[
E_{KS} \left[ \{ \phi \}_{i=1}^{N} \right] = \sum_{i,j=1}^{N} (S^{-1})_{ij} \int_{\Omega} \phi_i(r) \Delta \phi_j(r) + F[\rho] + \sum_{i,j=1}^{N} (S^{-1})_{ij} \int_{\Omega} \phi_i(r)(V_{\text{ext}} \phi_j)(r)
\]

\[
\rho(r) = \sum_{i,j=1}^{N} (S^{-1})_{ij} \phi_i(r) \phi_j(r)
\]

To take into account non-orthogonality

- Assume finite gap \( \varepsilon_N < \varepsilon_{N+1} \)
- Assuming functions \( \phi_i \) are linearly independent...
- No need for any eigenvalue computation!
DFT O(N) algorithm for localized functions

- Real-space (finite difference) discretization
- Norm-conserving pseudopotentials
- Parallel domain decomposition
- Confine functions to finite spherical regions
  - Each $\Phi_i$ lives on Finite Difference mesh, in a localization region of center $R_i$ and radius $R_c$
  - $O(1)$ d.o.f. for each orbital
- Iterative solver: direct minimization of energy functional
  - follow preconditioned steepest descent directions + block Anderson extrapolation scheme [JLF, J. Comp Phys 2010]
There remains an $O(N^3)$ operation…

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\]

\[
\rho(r) = \sum_{i,j=1}^{N} (S^{-1})_{ij} \phi_i(r) \phi_j(r)
\]

- Not even expensive, but requiring a lot of communications
  - $O(N^3)$ solver becomes a bottleneck beyond 10,000 atoms and/or 10,000 MPI tasks
- Smaller size than in Tight-Binding models or LCAO methods
- “Global” coupling
- Need to calculate selected elements of the inverse of Gram matrix $S$
- We essentially need the elements $S^{-1}_{ij}$ s.t. $S_{ij} \neq 0$
Gram (overlap) Matrix Properties

\[ S_{ij} = \int_\Omega \phi_i(r) \phi_j(r) \, dr \]

- \( S_{ij} = 0 \Rightarrow |\tilde{c}_i - \tilde{c}_j| > 2R_c \)
- \( \tilde{c}_i = \text{position of } \phi_i \)
- \( R_c = \text{local function radius} \)

- S is sparse, Symmetric Positive Definite
- Condition number is independent of problem size!!
- Inverse
  - In principle full matrix…
  - …But off-diagonal elements decay exponentially fast
    [Demko et al., Math. Comp. 1984] [Benzi & Razouk, ETNA 2007]
  - Assumption: spectrum of S bounded away from 0, independently of N
We verify fast exponential decay of off-diagonal elements of the inverse of Gram matrix

- Polymers, 1888 atoms
- How to make efficient use of it on large parallel computers?
O(N) short-range calculation of selected elements of $S^{-1}$

- Based on the approximate inverse strategy

$$\text{Solve: } \arg\min_{M \in \mathbb{R}^{N \times N}} \|SM - I\|_F \Rightarrow M \approx S^{-1}, I = \text{identity matrix}$$

- Sparsity pattern of $M$ is predetermined by geometric distance

$$\forall \phi_j \mid \bar{c}_j \in \Omega_L, \text{define } \mathcal{J} = \left\{ k \mid |\bar{c}_j - \bar{c}_k| < R_s \right\}$$

and set $M_{jk} \neq 0 \forall k \in \mathcal{J}$, for some distance $R_s$

- $R_s$ determines accuracy of selected elements of the inverse
Computations of selected elements boils down to inverting local principal submatrix

- Include rows and columns of $S$ corresponding to closest local functions (distance between centers)
- Solve for column $k$ using $\text{ILU0–preconditioned GMRES}$
- Note: $S$ not close to Identity matrix!!! (unlike in Tight-Binding or LCAO approach where no preconditioner is needed [Stechel et al. PRB 1994])
Error on approximate inverse decays fast with principal submatrix size

Example: polymer
Data layout

- Localized orbital are distributed across processors
- Each MPI task owns pieces of several functions
- Each MPI task computes partial contribution to the global matrices (overlap,...)
Exploiting sparsity poses challenges for fast parallel implementation compared to $O(N^3)$ algorithms

- Energy can be written as:
  \[ E_{ks} = Tr(S^{-1}H_\phi) + F(\rho), \text{ where } H_\phi = \Phi^T H \Phi \]

- $S^{-1}$ is approximated, sparse and has complete but distributed entries

- $H_\phi$ is sparse and distributed (incomplete entries)

- Each PE only needs entries corresponding to locally centered functions
  - Need to consolidate partial contributions of $H_\phi$

- Efficient data communication and assembling algorithm is needed
Parallel data communication / matrix assembly is key to efficiency

- Each parallel task computes partial contributions to some matrix elements.
- Need to assemble local principal submatrix matrix.
  - Sum up partial dot products computed on various processors.
- We use a short range communication pattern where data is passed down to nearest neighbor only, one direction at a time, for as many steps as needed.
- Overlap communication and computation.
  - Accumulate received data in sparse data structure while sending data for the next step.
- Need to scatter results to adjacent processors that need column $j$ of $S^{-1}$.
Three parameters to control error and achieve needed accuracy

- Finite difference Mesh spacing
  - error $O(h^4)$

- 2 parameters to control $O(N)$ truncation

  Localization of functions $\phi$

  Cutoff for $S^{-1}$ ($R_c=9$ Bohr)
Weak scaling: Test application

- Liquid water
  - 1536 atoms (512 molecules)
  - 2048 orbitals

- Replicate
  - 2x2x2
  - 3x3x3
  - 4x4x4
  - ...
Numerical results show excellent weak scaling and fast time to solution (No limit to scaling – in principle)
At 100K MPI tasks and beyond, everything needs to be distributed!

Liquid water on IBM/BGQ
Nearsightedness principle for parallel computation

- W. Kohn’s nearsightedness principle [PRL 1996]
- Nearsightedness in computational algorithm leads to $O(N)$ and parallel scaling beyond 100,000 MPI tasks
  - Practical accuracy achieved with short range communications / no global communications for insulators
Conclusion

- Research supported by LLNL LDRD program
- Recent Publications
  - D. Osei-Kuffuor and JLF, PRL 2014
- Future
  - Speed-up time-to-solution (threading)
  - Applications
    - Distribution of ions in dilute solution: K + Cl in water
    - Biology
  - Extension to metals…