DL_MG: Solving the Poisson equation made easy!
A parallel multigrid solver library for electronic structure calculations in vacuum and solution

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Preamble

Slides will soon be available at jcwomack.com

Bibliographic references — ask me, or see slides online
The Poisson equation in electronic structure

\[
\left( -\frac{1}{2} \nabla^2 + \hat{V}_{\text{eff}} \right) \psi_i = \varepsilon_i \psi_i
\]

\[
E_{\text{KS}}[n] = T_s[n] + E_{\text{es}}[n] + E_{\text{xc}}[n]
\]
The Poisson equation in electronic structure

\[ E_{es}[n] = \frac{1}{2} \int d\mathbf{r} \, n(\mathbf{r}) \phi_0[n](\mathbf{r}) \]

\[ \nabla^2 \phi_0(\mathbf{r}) = -4\pi n(\mathbf{r}) \]

\[ \tilde{\phi}_0(\mathbf{G}) = 4\pi \frac{\tilde{n}(\mathbf{G})}{|\mathbf{G}|^2} \]

Standard Poisson equation (SPE)
- Vacuum or uniform permittivity
- Potential \( \phi_0 \) due to charge density \( n \)

Analytic reciprocal space solution
- Under fully periodic BCs
- \( n \) must be neutral, i.e. \( \tilde{n}(0) = 0 \)
Continuum dielectric implicit solvent models

- Place charge density in vacuum cavity
- Embed in polarizable dielectric medium
- Solve for $\phi$ using the...

**Generalized Poisson equation (GPE)**

$$\nabla \cdot (\varepsilon(\mathbf{r}) \nabla \phi(\mathbf{r})) = -4\pi n(\mathbf{r})$$

- Non-homogeneous permittivity $\varepsilon$
- $\phi$ includes effect of polarizing dielectric medium, i.e. $\phi = \phi_0 + \phi_r$
The minimal parameter implicit solvent model (MPSM)

- In ONETEP [1, 2] and CASTEP [3]
- Refinement of earlier work by Fattebert, Gygi and Scherlis [4, 5]

Smoothly varying dielectric function

\[
\varepsilon(\mathbf{r}) = 1 + \frac{\varepsilon_\infty - 1}{2} \left( 1 + \frac{1 - (n_{\text{elec}}(\mathbf{r})/n_0)^{2\beta}}{1 + (n_{\text{elec}}(\mathbf{r})/n_0)^{2\beta}} \right)
\]

- Defined in terms of electron density
- Two fitted parameters: \( n_0, \beta \)
- Yields a continuous potential \( \phi \)

Note: There are many more details to this model (e.g. non-electrostatic part, BCs, ionic charge) — see papers of Dziedzic et al. for full description [1, 2].
Free energies of solvation computed with the MPSM and other models

<table>
<thead>
<tr>
<th>Approach</th>
<th>XC functional</th>
<th>RMS error</th>
<th>Max error</th>
<th>$R$</th>
</tr>
</thead>
<tbody>
<tr>
<td>MPSM$^a$</td>
<td>PBE</td>
<td>3.8</td>
<td>8.3</td>
<td>0.83</td>
</tr>
<tr>
<td>MPSM$^b$</td>
<td>PBE</td>
<td>4.1</td>
<td>9.1</td>
<td>0.83</td>
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<tr>
<td>PCM</td>
<td>PBE</td>
<td>10.9</td>
<td>23.3</td>
<td>0.53</td>
</tr>
<tr>
<td>SMD</td>
<td>M05-2X</td>
<td>3.4</td>
<td>14.5</td>
<td>0.87</td>
</tr>
<tr>
<td>AMBER</td>
<td>(classical)</td>
<td>5.1</td>
<td>19.9</td>
<td>0.77</td>
</tr>
</tbody>
</table>

$^a$ With cavity responding self-consistently to changes in density.

$^b$ With cavity fixed.

The MPSM performs as well, if not better than other models, with only 2 fitted parameters!

Accuracy is important, but so are performance and efficiency!

An efficient GPE solver is needed...

- 71 neutral molecules in H$_2$O [6, 7]
- Errors (kcal mol$^{-1}$) wrt experimental free energies of solvation [8]
- See original MPSM paper [1]
DL_MG: An overview

A flexible, scalable, and accurate open source Poisson solver library

- Parallel (MPI + OpenMP) multigrid approach [9]
- Written in modern Fortran
- SPE, GPE, and Poisson-Boltzmann equation
- Periodic, open and mixed BCs
- High-order accuracy via iterative defect correction [9, 10].

- Used extensively in ONETEP for implicit solvent calculations
- Available from www.dlmg.org now!
Solver implementation: Multigrid

Discretized Poisson equation

\[ \hat{A}_h u_h = f_h \]

- \( \hat{A} \) is \( \nabla^2 \) or \( \nabla \cdot \varepsilon(\mathbf{r}) \nabla \)
- \( u \) is the potential, \( \phi(\mathbf{r}) \)
- \( f \) is the charge density, \( n(\mathbf{r}) \)

Solvable by stationary iterative methods:

- High frequency components of the error are rapidly attenuated
- But low frequency components limit convergence

Multiple grids can improve convergence:

- On a coarser grid, lower frequency components appear higher in frequency
- Correct the solution on a fine grid using error from a coarser grid
- Apply recursively on grid hierarchy
Solver implementation: High-order defect correction

- Initial solution is obtained using a 2\textsuperscript{nd}-order multigrid solver
- Discretization error reduced using high-order defect correction method [9, 10]

```
1: \( i = 0 \)
2: Solve \( \hat{A}_2 u^{(0)} = f \)
3: \textbf{while} not converged \textbf{do}
4: \hspace{1em} Compute \( r_d^{(i)} = f - \hat{A}_d u^{(i)} \)
5: \hspace{1em} Solve \( \hat{A}_2 e_{2,d}^{(i)} = r_d^{(i)} \)
6: \hspace{1em} Correct \( u^{(i+1)} = u^{(i)} + e_{2,d}^{(i)} \)
7: \hspace{1em} \( i = i + 1 \)
8: \textbf{end while}
```

- High-order operator \( \hat{A}_d \) is only needed to compute \( r_d \) on the fine grid
- Multigrid can use a simpler \( \hat{A}_2 \) operator
- ...then correct to higher-order accuracy

By employing this scheme, we avoid the complexity of applying high-order operators on coarse grids.
Accuracy of the solver with order of finite differences

- DFT (ONETEP) with DL_MG
- 448 atom graphene sheet
- Solving the SPE in periodic BCs

\[ \nabla^2 \phi_0(r) = -4\pi n(r) \]

- Error is wrt analytic solution
- Sub-\(\mu E_h/\)atom error for \(\geq 10^{\text{th}}\)-order FD

High-order defect correction reduces the error by orders of magnitude!
Scaling of computational work with problem size

- Solving the GPE for a simple model
- Gaussian $\phi(\mathbf{r})$, erf-derived $\varepsilon(\mathbf{r})$
- Represents an isolated molecule embedded in implicit solvent [12]

$$\nabla \cdot (\varepsilon(\mathbf{r})\nabla \phi(\mathbf{r})) = -4\pi n(\mathbf{r})$$

- Useful for benchmarking:
  1. Can arbitrarily scale grid size
  2. Analytic solution is known

We observe $O(N_{\text{grid}})$ scaling in all components up to $\sim 1000^3$ gridpoints!

Run on MMM Hub “Thomas”: 6 nodes/64 MPI processes & 2 OpenMP threads per MPI
A very brief introduction to DL_MG’s API

Initialization

```call dl_mg_init(nx, ny, nz, dx, dy, dz, bc, gstart, gend, &
    mg_comm, report_unit, report_file, ierr)``

Calling the solver

```call dl_mg_solver(eps, eps_mid, alpha, rho, &
    pot, fd_order, ierr)```  

Simple, yet powerful:

- Sensible default algorithms and parameter values
- Expert users can tune these via optional arguments
- Equation type is inferred from arguments to overloaded `dl_mg_solver`
Summary

DL_MG: Solving the Poisson equation made easy!

1. A flexible, scalable and accurate Poisson solver library

2. Enables electronic structure calculations in vacuum and solvent

3. Simple, yet powerful API
# Acknowledgements

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## Collaborators

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- Phil J. Hasnip (York)
- Matt I. J. Probert (York)
- Chris-Kriton Skylaris (Southampton)
Further information

www.dlmg.org

Paper

*DL_MG: A Parallel Multigrid Poisson and Poisson–Boltzmann Solver for Electronic Structure Calculations in Vacuum and Solution*
J.C. Womack, L. Anton, J. Dziedzic, P.J. Hasnip, M.I.J. Probert, and C.-K. Skylaris,

Technical report

*Implementation and Optimisation of Advanced Solvent Modelling Functionality in CASTEP and ONETEP*
J.C. Womack, L. Anton, J. Dziedzic, P.J. Hasnip, M.I.J. Probert, and C.-K. Skylaris,
*ARCHER eCSE technical report* eCSE07-006 (2017)
Strong scaling of DL_MG when solving the GPE

- Solving the GPE for a simple model
- Gaussian $\phi(r)$, erf-derived $\varepsilon(r)$
- Fixed problem size: $N_{\text{grid}} = 1089^3$
- 1, 2 of 4 OpenMP threads per MPI
- Reported speed up is for the minimum total time over 5 repetitions
- Run on MMM Hub “Thomas” supercomputer

Near linear, but less-than-ideal, speed up for typical core counts used in parallel electronic structure calculations (10s to 100s of cores).
Bibliography I


