A Method for Solving Poisson Problems

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The Electrostatic Potential

In this work, we are developing a stable, accurate, and fast method for calculating the electrostatic potential on a grid. We calculate it by using the operator solution to the Poisson equation:

$$V(\mathbf{x}) = \frac{2\pi\hbar^2}{m_0}\hat{T}^{-1}\rho_0(\mathbf{x})$$

$\rho_0(\mathbf{x})$: charge distribution

$\hat{T}$: the kinetic energy operator for a fictitious particle of mass m_0

Using the identity $\hat{T}^{-1} = \int_0^\infty \mathrm{d}\beta e^{-\beta\hat{T}}$ we obtain

$$V(\mathbf{x}) = \int_0^\infty \mathrm{d}\beta \int_{\mathbb{R}^3} \mathrm{d}\mathbf{x}' \left\langle \mathbf{x} \middle| e^{-\beta\hat{T}} \middle| \mathbf{x}' \right\rangle \psi_0(\mathbf{x}')$$

$$\psi_0(\mathbf{x}) \equiv \frac{2\pi\hbar^2}{m_0}\rho_0(\mathbf{x})$$

The Integration Technique

For the integral over $\mathbb{R}^3$

C. Predescu, *J. Theor. Comp. Chem.* **5**:255, 2006.

$$\psi_\tau(x,y,z) = \sum_{j_x,j_y,j_z=-1}^{1} w^h_{j_x} w^h_{j_y} w^h_{j_z} \psi_0(x+j_x\Delta, y+j_y\Delta, z+j_z\Delta)$$

$$\Delta = h\sigma \qquad h = \sqrt{3} \qquad w^h_{-1} = w^h_1 = 1/6 \qquad w^h_0 = 2/3$$

For the integral over β

$$V(\mathbf{x}) = \int_0^\tau \mathrm{d}\beta\psi_\beta(\mathbf{x}) + \int_\tau^\infty \mathrm{d}\beta\psi_\beta(\mathbf{x})$$

$$= \int_0^\tau \mathrm{d}\beta\psi_\beta(\mathbf{x}) + \left(e^{-\tau\hat{T}}V\right)(\mathbf{x})$$

$$\psi_\beta(\mathbf{x}) = \int_{\mathbb{R}^3} \mathrm{d}\mathbf{x}' \left\langle \mathbf{x}\middle| e^{-\beta\hat{T}} \middle|\mathbf{x}'\right\rangle \psi_0(\mathbf{x}')$$

Features of the technique

- This technique is stable (positive charge distributions will produce positive potentials at all levels of approximation).
- Because of the iterative nature of this technique, we can use an initial guess potential instead of the initial charge distribution in order to speed up the computation.
- We also avoid the need for excessively large grids by using Beck's suggestion to calculate the potential on the frontier exactly.
- The technique is parallelizable on distributed memory machines with preservation of scaling (domain decomposition).

T. L. Beck. *Rev. Mod. Phys.* **72**:1041, 2000.

Discrete Charge Distributions

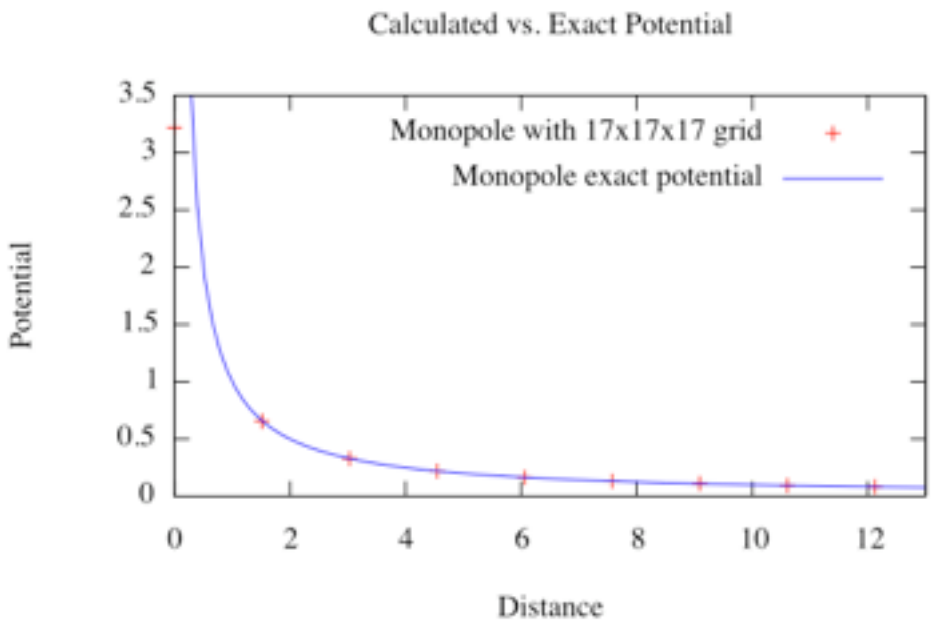
To test this technique, several discrete charge distributions have been used. A simple monopole, with charge +1.0, is the first example. Because the $1/r$ fall-off of the monopole potential is extremely slow, this is expected to be the worst-case scenario for this technique.

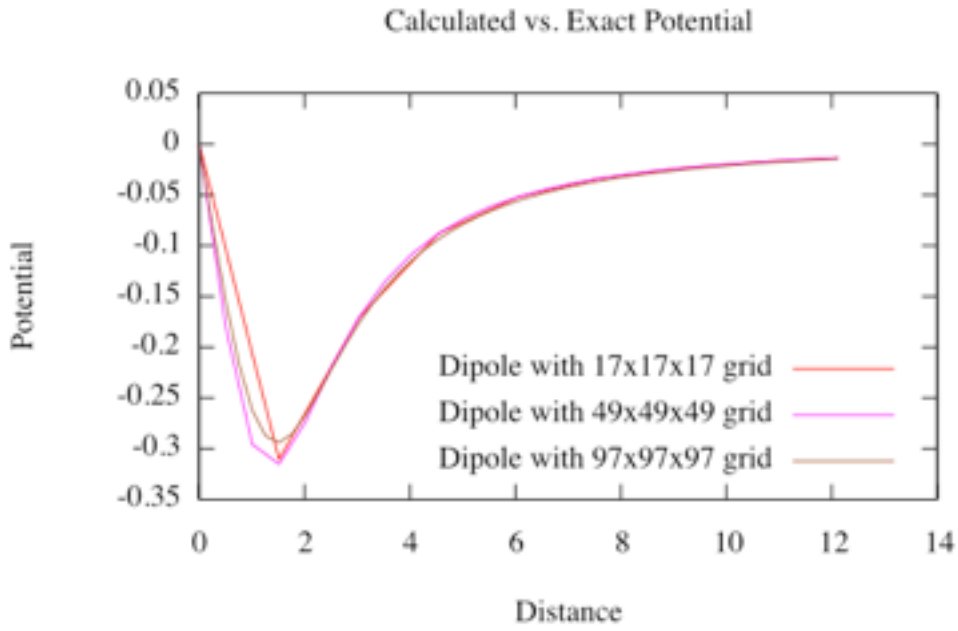
Dipoles have also been studied, with unit charges of opposite sign separated by 2.0 units of distance. Larger separations were also explored with essentially the same results.

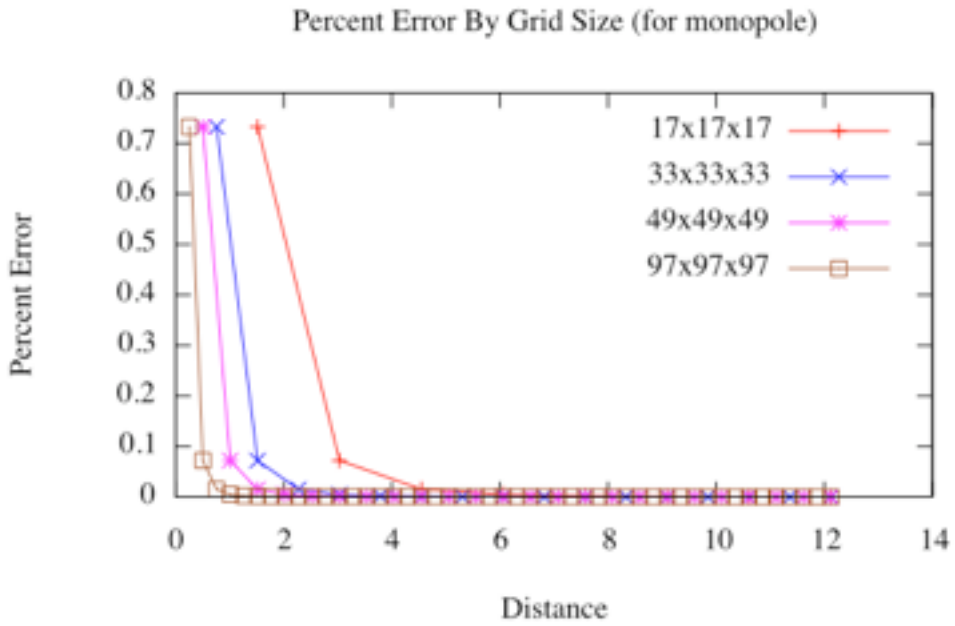
Finally, a quadrupole with a positive central charge (+2.0) and negative unit charges at 1.0 units from the center was studied.

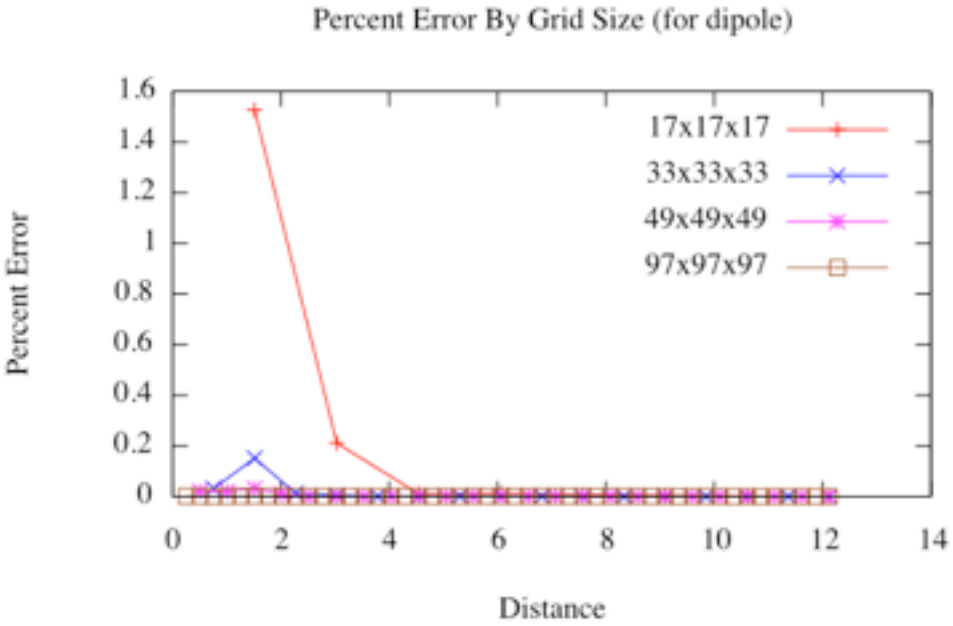
All of these systems were studied in a cube with side length 15.0 units, with 17^3, 33^3, 49^3, 65^3, 81^3, and 97^3 total gridpoints.

Accuracy of the Technique

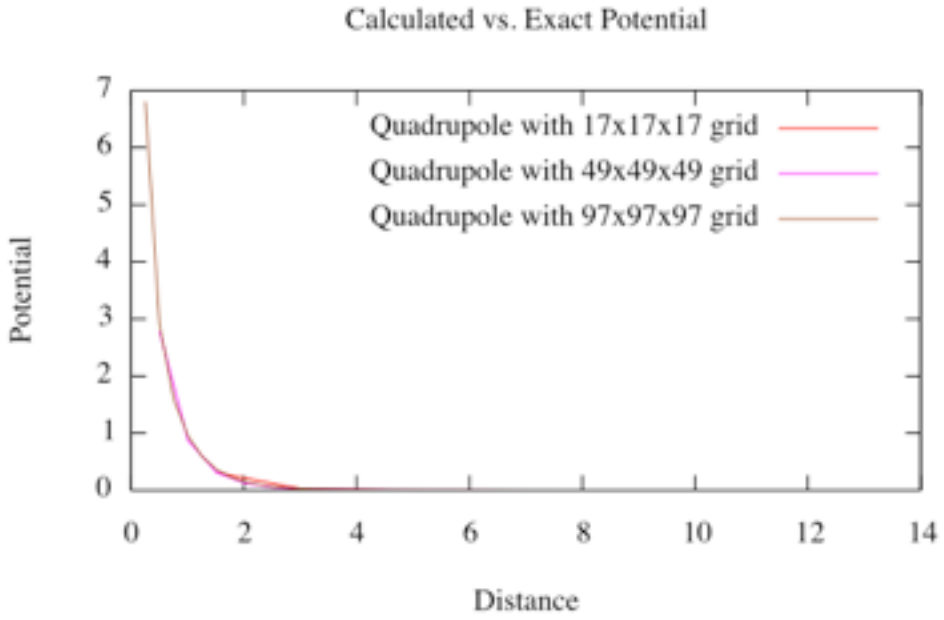


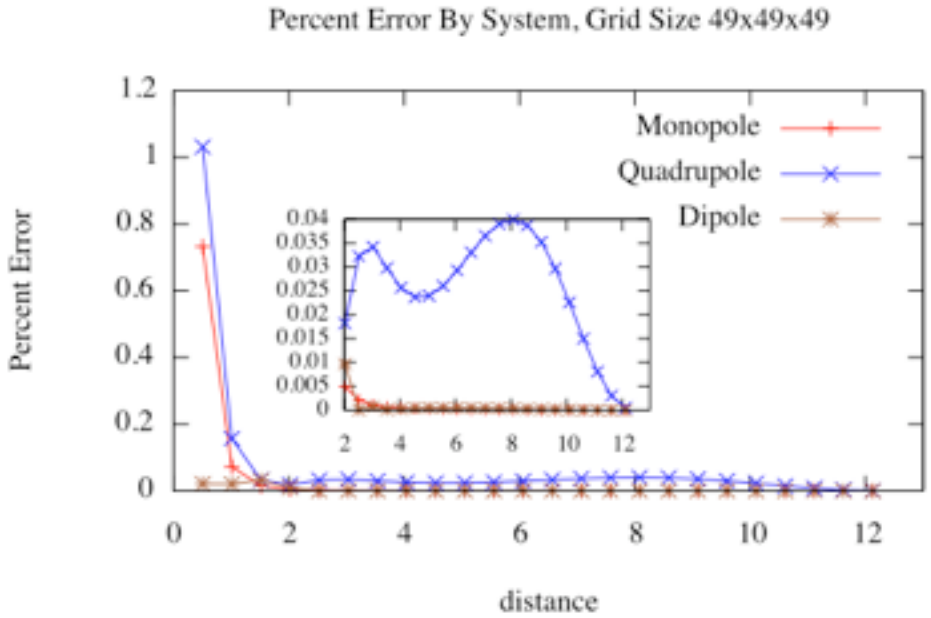


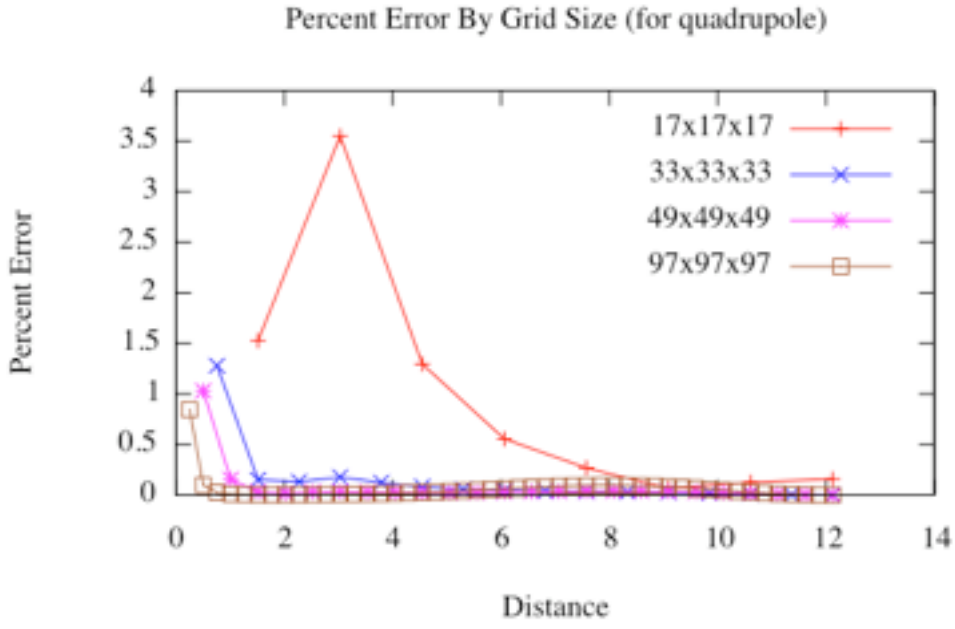


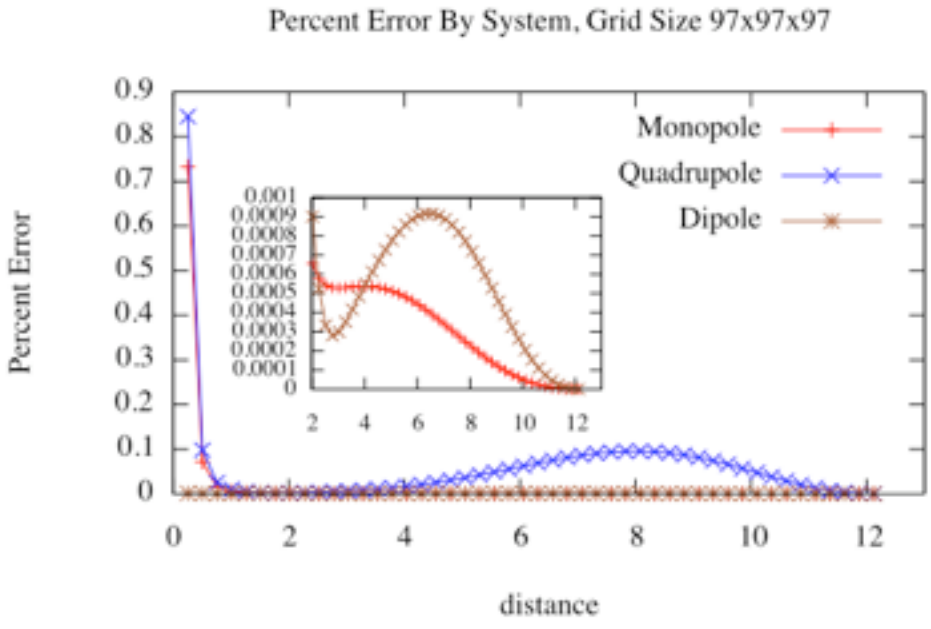


Accuracy

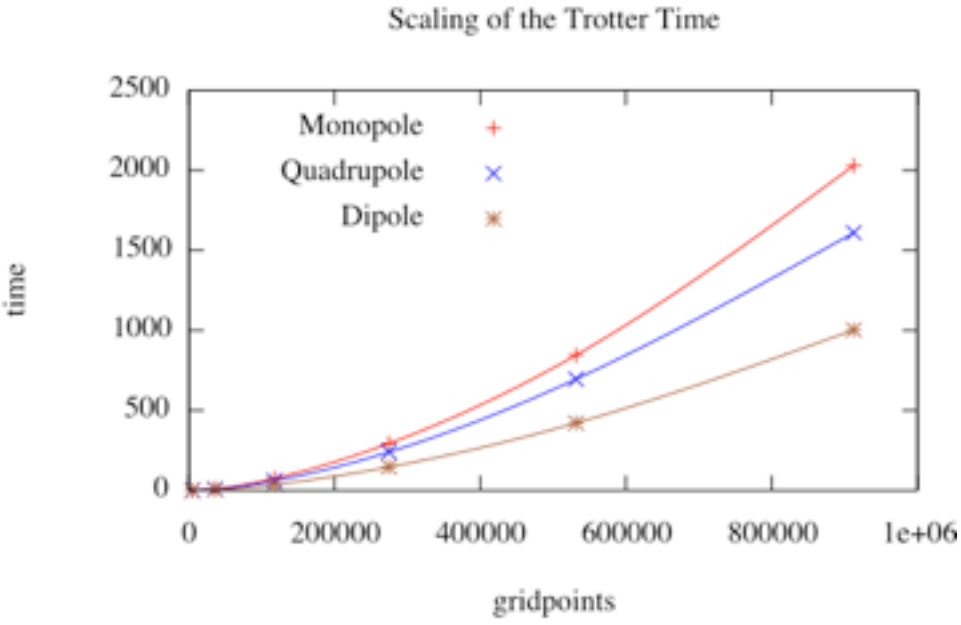

Calculated vs. Exact Potential
Quadrupole with 17x17x17 grid
Quadrupole with 49x49x49 grid
Quadrupole with 97x97x97 grid
Potential
Distance

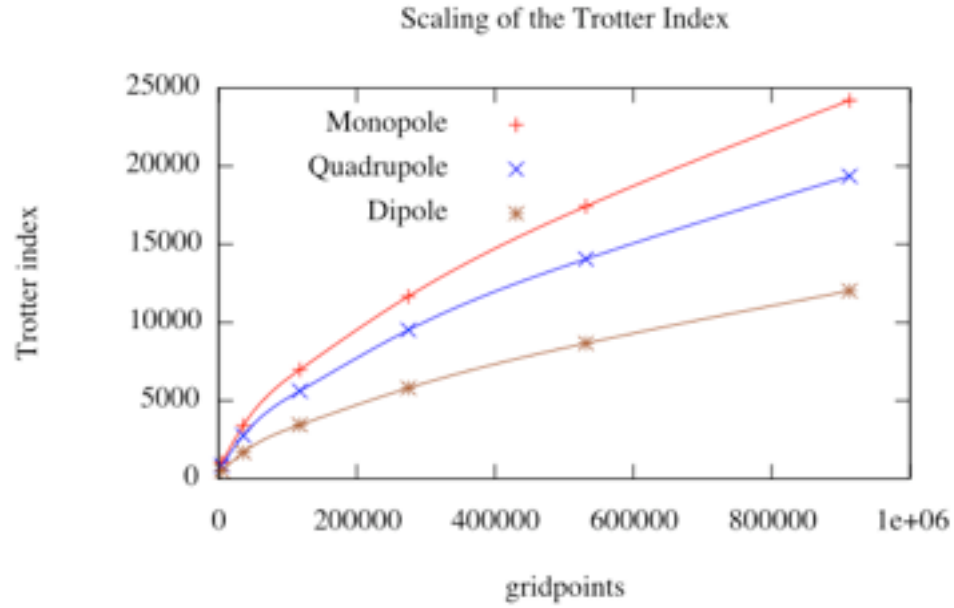

Percent Error By System, Grid Size 49x49x49
Monopole
Quadrupole
Dipole
Percent Error
distance


Percent Error By Grid Size (for quadrupole)
17x17x17
33x33x33
49x49x49
97x97x97
Percent Error
Distance


Percent Error By System, Grid Size 97x97x97
Monopole
Quadrupole
Dipole
Percent Error
distance

Timing of the Technique





The timing of this technique has been explored in what is expected to be the worst case scenario. The "guess" potential is set to the charge distribution. The convergence criterion was a maximum change of 10^{-8} over ten Trotter steps.

Both the Trotter iteration and the calculation of the exact values on the frontier take $O(n^{5/3})$ time. However, the calculation of the frontier (naïvely implemented) takes 2 or 3 times as long as the Trotter iteration (converging to 10^{-8}) in measured CPU time.

As expected, the monopole gives the slowest convergence, because of its long-range effects. The dipole converges fastest.

Future Directions

- Application of fourth-order integration techniques for improved accuracy
- Use of guess potentials to decrease number of iterations required for convergence
- Explore use of multigridding with this technique
- This technique is a step in a larger project to use the density matrix formalism for linearly scaling electronic structure calculations

We would like to acknowledge useful discussions with William H. Miller and the NSF and ONR for funding. We would also like to acknowledge NERSC for computer time.