A Low-Communication Method to Solve Poisson's Equation on Locally-Structured Grids

Peter McCorquodale (PWMcCorquodale@lbl.gov), Phillip Colella (PColella@lbl.gov), Brian Van Straalen (BVVanstraalen@lbl.gov), Lawrence Berkeley National Laboratory; Christos Kavouklis (kavouklis1@llnl.gov), Lawrence Livermore National Laboratory

Continuous Problem and Solution

Poisson's equation arises in such fields as astrophysics, plasma physics, electrostatics, and fluid dynamics. We are solving it with infinite-domain boundary conditions:
\[ \Delta \phi = f, \]
\[ \phi(x) = \int \frac{f(y)dy}{|x-y|} + \alpha \quad \text{as} \quad |x| \rightarrow \infty \]
Solution of this equation, with Green's function, \( G \):
\[ \phi(x) = (G \ast f)(x) = \frac{1}{4\pi} \int_{|y|<\Delta} f(y) dy \]

Method of Local Corrections (MLC)

Represent potential \( \phi \) as linear superposition of small local discrete convolutions, with global coupling represented using a non-iterative form of geometric multigrid.
Communication cost like that of a single level of multitigrid.
Computational kernels are multidimensional FFTs on small domains.

Local Discrete Convolutions

We can compute infinite-domain discrete Green's function \( G \) on any finite domain at any mesh resolution. We compute \( G \) once, store, and scale for any \( \Delta \).
\[ (\Delta \ast G^{\Delta=\Delta})(x) = \begin{cases} \frac{1}{|x-y|}, & y=0, \\ 0, & \text{otherwise}. \end{cases} \]
\[ G^{\Delta=\Delta}(x) = (\Delta^{-1} f)(x) \quad \text{fast convolution using 3D FFT} \]
Scaling: \( G^{\Delta} |h| = h^{-1} G^{\Delta=\Delta} |g| \)
\( (G^{\Delta} \ast f^{\Delta})(|g|) = \sum_{l,d} h^{d} G^{\Delta=\Delta}(g_{l}) \cdot f^{\Delta}(l,\theta^{d}) \)

MLC Algorithm Description

Domain decomposition strategy:
2 grid levels, fine (spacings \( h \)) and coarse (spacings \( H \)), with \( h/H = 4 \) fixed. Decompose fine domain into fixed-sized patches of radius \( R = (N-1)/2 \), where \( N \) is number of grid points along each dimension.
1. For each fine patch of radius \( R \), compute local convolutions on patches of radius \( hR \):
   \[ \phi^{hR} = G^{hR} \ast f^{hR} \]
   - on patch \( i \) expanded by factor \( a \)
   - Example: patch in red
   - blue dashed line around patch \( i \)
2. Accumulate coarse-grid right-hand side by summing up localized contributions:
   \[ f^{H} = \sum_{l,d} (C_{\text{assemble}}(\phi^{hR})) \]
3. Compute global coarse convolution:
   \[ f^{H} = G^{H} \ast f^{H} \]
4. On each patch, solve a Dirichlet problem for Poisson, with face values
   \[ \phi^{hR} = \sum_{l,d} C_{\text{assemble}}(\phi^{hR}) \]

High-Order Mehrstellen Stencils

A discrete Laplacian stencil of radius \( s \) has form
\[ (\Delta^{s} \phi)^{h} = \sum_{k=-l}^{l} a_{k} \phi^{h}_{s+k} \]
and truncation error looks like:
\[ \Delta^{s} \phi - \Delta \phi = C^{h}_{s} \Delta(\phi) + \sum_{k=2}^{l} h^{2s} \sum_{(l,q)} C^{(l,q)}(s)(\phi_{q}^{h} + O(h^{2s+2})) \]
constant
stencil radius \( s \):
- 27-point operator: \( s = 1, q = 6, C = 11/2 \)
- 117-point operator: \( s = 2, q = 10, C = 11/2 \)

Modifying right-hand side of \( \Delta \phi = f \) by adding appropriate derivatives of \( f \) gives a high-order approximation with compact stencil \( \Delta^{s} \phi \)
(And for \( \phi \) harmonic, truncation error is \( O(h^{2s}) \) without modifying right-hand side.)

Solution Error

\[ \phi^{\text{MLC}} - \phi = O(h^{N_{\Delta}}) + \frac{f}{\| f \|_{\infty}} O \left( \frac{H}{\alpha N_{\Delta}} ight)^{Q} \]
From local truncation error, depends on local derivatives of \( f \) and number of terms in Mehrstellen correction of right-hand side.
Typically \( q = 4 \) or 6.

Modifying for Efficiency at Finest Level

At finest level only, reduce cost of computing local convolutions by replacing them on an outer annulus with fields induced by Legendre expansions of order \( P \):
- Red + inner white (\( \beta \)) region: \( C^{\beta} \ast f^{\beta} \)
- Gray (\( \alpha \) + \( \beta \)) region: \( C^{\alpha} \ast f^{\alpha} \)
Precompute convolutions of \( C^{\alpha} \) with Legendre polynomials, and communicate only the coefficients for this region. Error is \( (N_{\Delta}^{2}) \).

Performance Analysis

Comparison with geometric multigrid (GMG) for 27-point Laplacian operator.
GMG with 10 V-cycles, vs. MLC with \( \alpha = 4, \beta = 6, N = 33, \alpha = 2.35, \beta = 2.25, P = 3 \).

Accuracy Tests

Use \( q = 4 \), patch size \( N \) either 33 or 65. We find error \( O(N_{\Delta}^{2}) \) down to a barrier.
Uniformly refined grids:
Adaptively refined grids:

Scaling Tests

on NERSC Cori (IHaswell)

Numerical parameters: \( q = 6, N = 33, \alpha = 2.35, \beta = 2.25 \). Plots of wall-clock time to solution (seconds).

Comparison with HPGMG

256 cores (8 nodes) on NERSC Cori I

- 6.1 sec for HPGMG with 10 V-cycles on uniform 1024\(^2\) grid (Sam Williams, private communication).
- 1.07 sec solve time for MLC on 10\(^3\) grid points adaptively distributed (0.2% of domain refined at finest level).

For More Information

- Our website: http://www.chombo.lbl.gov

Acknowledgments: This research was supported at the Lawrence Berkeley National Laboratory by the Office of Advanced Scientific Computing Research of the U.S. Department of Energy under Contract No. DE-AC02-05CH11231.