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

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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**:

$$\Delta\phi = f\ , \qquad \phi(\boldsymbol{x}) = -\frac{1}{4\pi|\boldsymbol{x}|}\int f(\boldsymbol{y})d\boldsymbol{y} + o\left(\frac{1}{|\boldsymbol{x}|}\right) \text{ as } |\boldsymbol{x}|\to\infty$$

Solution of this equation, with Green's function, G:

$$\phi(\boldsymbol{x}) = (G*f)(\boldsymbol{x}) \equiv \int G(\boldsymbol{x}-\boldsymbol{y})f(\boldsymbol{y})\,d\boldsymbol{y}\ ,\ G(\boldsymbol{z}) = -\frac{1}{4\pi|\boldsymbol{z}|}.$$

Method of Local Corrections (MLC)

Represent potential ϕ 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* iteration of multigrid.

Computational kernels are multidimensional FFTs on small domains.

Local Discrete Convolutions

We can compute infinite-domain discrete Green's function G^h on any finite domain at any mesh resolution h. Compute $G^{h=1}$ once, store, and scale for any h.

$$(\Delta^{h=1}G^{h=1})[\boldsymbol{g}] = \begin{cases} 1, \text{if } \boldsymbol{g}=\boldsymbol{0}; \\ 0, \text{otherwise.}\end{cases} \qquad (G^h * f^h) = (\Delta^h)^{-1}(f^h)$$

fast convolution using 3D FFT

Scaling: $G^h[\boldsymbol{g}] = h^{-1}G^{h=1}[\boldsymbol{g}]$ $\qquad (G^h*f^h)[\boldsymbol{g}] \equiv \sum_{\boldsymbol{g}'\in\mathbb{Z}^3} h^3 G^h[\boldsymbol{g}-\boldsymbol{g}']f^h[\boldsymbol{g}']$

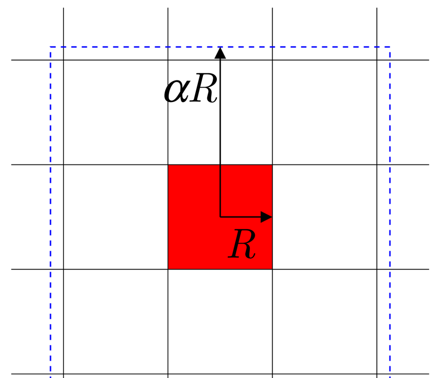
MLC Algorithm Description

Domain decomposition strategy:
2 grid levels, fine (spacing h) and coarse (spacing H), with H/h = 4 fixed.
Decompose fine domain into fixed-sized patches of radius $R = (N\text{-}1)h/2$,
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 αR:

$$\phi_k^{h,\text{init}} = G^h * f_k^h$$

on patch k expanded by factor α — *on patch k*



Example:
- patch k in red;
- blue dashed line around patch k expanded by factor of α = 3.25

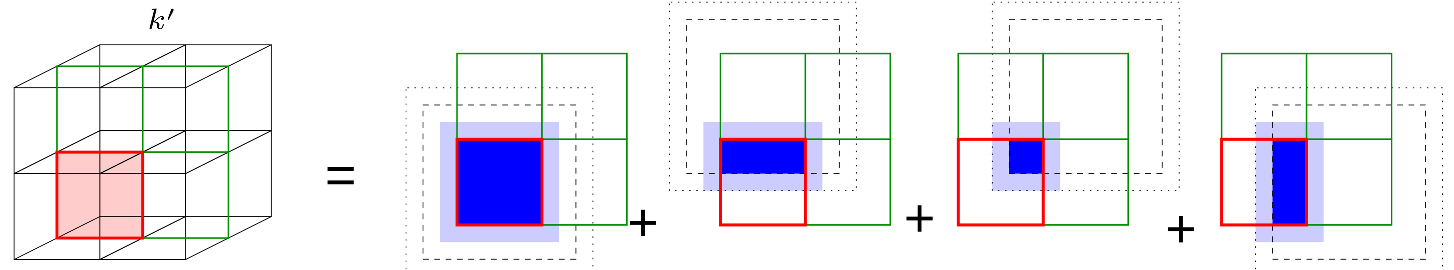
2. Accumulate coarse-grid right-hand side by summing up localized contributions:

$$F^H = \sum_k \Delta^H(\text{Coarsen}(\phi_k^{h,\text{init}}))$$

3. Compute global coarse convolution: $\phi^H = G^H * F^H$

4. On each patch, solve a Dirichlet problem for Poisson, with face values

$$\phi_k^h = \sum_{k'}\phi_{k'}^{h,\text{init}} + \text{Interp}(\phi^H - \sum \text{Coarsen}(\phi_{k'}^{h,\text{init}}))$$



Boundary values on the red face of patch k: contributions from $\phi_{k'}^{h,\text{init}}$ on dark blue regions, $\text{Coarsen}(\phi_{k'}^{h,\text{init}})$ interpolated from light blue regions.

For more than 2 levels, apply the above algorithm recursively.

High-Order Mehrstellen Stencils

A discrete Laplacian stencil of radius s has form $\quad (\Delta^h\phi^h)_{\boldsymbol{g}} = \sum_{\boldsymbol{s}\in[-s,s]^3} a_{\boldsymbol{s}}\phi^h_{\boldsymbol{g}+\boldsymbol{s}}$

and truncation error look like:

$$\Delta^h\phi^h - \Delta\phi = \underbrace{C_2}_{\text{constant}} h^2\Delta(\Delta\phi) + \sum_{Q'=2}^{Q/2-1} h^{2Q'}\underbrace{\mathcal{L}^{2Q'}}_{\text{order } 2Q'}(\Delta\phi) + h^Q\underbrace{\mathcal{L}^{Q+2}}_{\text{order } Q+2}(\phi) + O(h^{Q+2})$$

linear differential operators

stencil radius $s = \left\lfloor \frac{Q}{4} \right\rfloor$

27-point operator: s = 1, Q = 6, C_2 = 1/12
117-point operator: s = 2, Q = 10, C_2 = 1/12

Modifying right-hand side of $\Delta\phi = f$ by adding appropriate derivatives of f gives a high-order approximation with compact stencil Δ^h.

(And for ϕ harmonic, truncation error is $O(h^Q)$ without modifying right-hand side.)

Solution Error

$$\phi^{\text{MLC}} - \phi = \underbrace{O(h^q)} + \underbrace{\|f\|_\infty O\left(\left(\frac{H}{\alpha Nh}\right)^Q\right)}$$

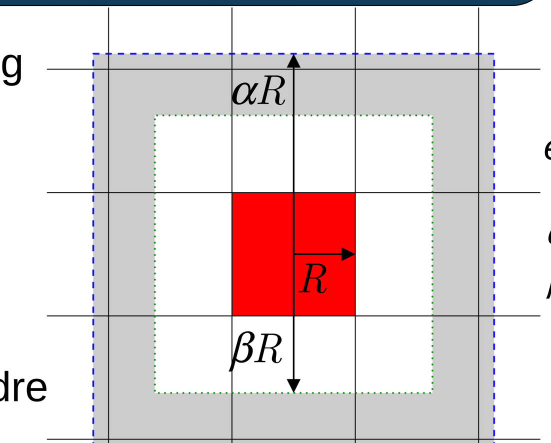
From local truncation error, depends on local derivatives of ϕ and number of terms in Mehrstellen correction of right-hand side.
Typically q = 4 or 6.

Localization error, from representation of smooth nonlocal coupling
- no dependence on derivatives
- $O(1)$ relative to h
- can adjust α, N, Q (stencil) as needed

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 (βR) region: $G^h * f^h$
- Gray ($\alpha R - \beta R$) region: $G^h * \text{Proj}_P(f^h)$

Precompute convolutions of G^h with Legendre polynomials, and communicate only the coefficients for this region. Error is $O(h^{P+1})$.



example with α = 3.25 β = 2.25

Performance Analysis

Comparison with geometric multigrid (GMG) for 27-point Laplacian operator.
GMG with 10 V-cycles, vs. MLC with q=4, Q=6, N=33, α=3.25, β=2.25, P=3.

Algorithm	flops per gridpoint	loads (in bytes) per gridpoint	stores (in bytes) per gridpoint	messages per phase
GMG	1210	3840	1920	20
MLC	4637+398=5035	344	351	2

step 1   *everything else*

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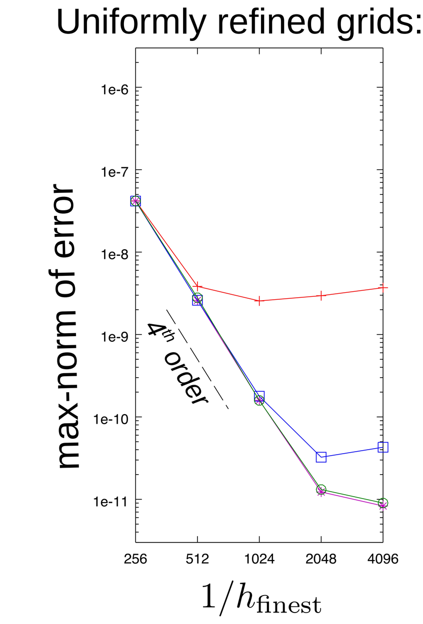
Accuracy Tests

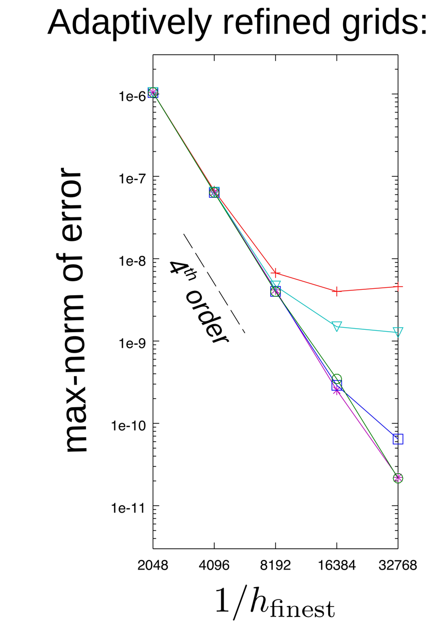
Use q=4, patch size N either 33 or 65. We find error $O(h^4_{\text{finest}})$ down to a barrier.

Uniformly refined grids:

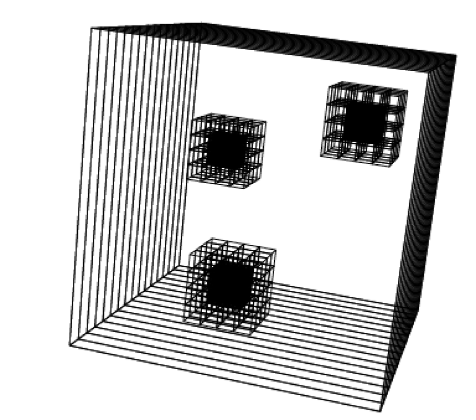


+: Q=6, α=3.25, N=33
□: Q=6, α=3.25, N=65
✳: Q=10, α=3.25, N=33
O: Q=10, α=3.25, N=65

Adaptively refined grids:



+: Q=6, α=3.25, N=33
▽: Q=6, α=2.125, N=65
□: Q=6, α=3.25, N=65
✳: Q=10, α=3.25, N=33
O: Q=10, α=3.25, N=65



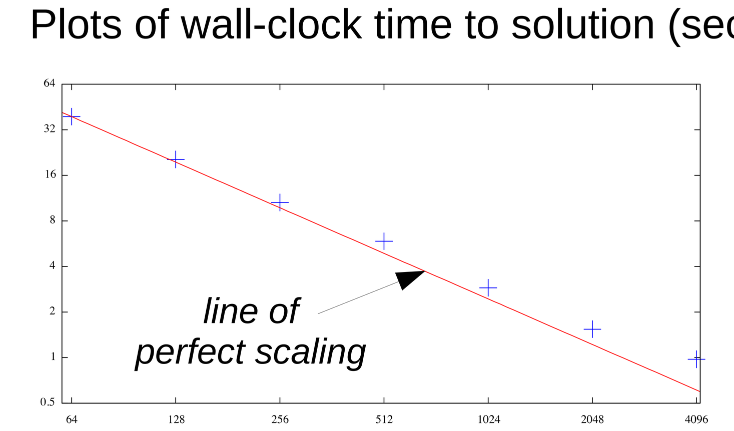
Test case with 3 spherical charges, adaptive grids shown above.

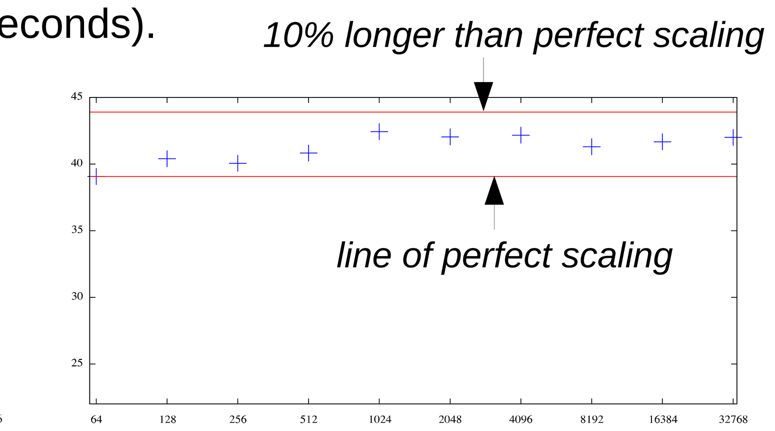
At finest level, project to Legendre polynomials of degree up to P=3.
α = 3.25 ⇒ β = 2.25;
α = 2.125 ⇒ β = 1.625.

Scaling Tests

on NERSC Cori I (Haswell)

Numerical parameters: Q = 6, N = 33, α = 3.25, with finest level β = 2.25.
Plots of wall-clock time to solution (seconds).





Strong scaling:
- fixed problem size with 10^9 grid points
- adaptive distribution (0.2% of domain refined at finest level)
- over range 64 – 4K cores, strong scaling efficiency > 60%
- time to solution 39.1 → .97 seconds

Replication weak scaling:
- adaptive base case with 10^9 grid points
- replicated to obtain larger problems on 64 – 32K cores
- solution error independent of scale (~7 x 10^{-9})
- 92% weak scaling efficiency
- time to solution 39.1 – 42.4 seconds
- largest calculation has 5.1 x 10^{11} unknowns, with equivalent uniform-grid resolution of $(64\text{K})^3$ = 2.8 x 10^{14} unknowns.

Comparison with HPGMG

256 cores (8 nodes) on NERSC Cori I

- 6.1 sec for HPGMG with 10 V-cycles on uniform 1024^3 grid (Sam Williams, private communication).
- 10.7 sec solve time for MLC on 10^9 grid points adaptively distributed (0.2% of domain refined at finest level).

For More Information

- C. Kavouklis and P. Colella, "Computation of Volume Potentials on Structured Grids Using the Method of Local Corrections", submitted to *Comm. App. Math. and Comp. Sci.*, also on `http://arxiv.org/abs/1702.08111`
- P. McCorquodale, P. Colella, G. T. Balls, and S. B. Baden, "A local corrections algorithm for solving Poisson's equation in three dimensions", *Comm. App. Math. and Comp. Sci.*, **2**:57—81 (2007).
- Our website `http://www.chombo.lbl.gov`