A Local Corrections Algorithm for Solving Poisson's Equation in Three Dimensions

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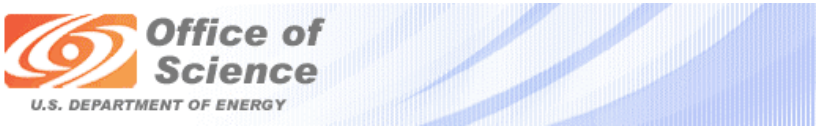


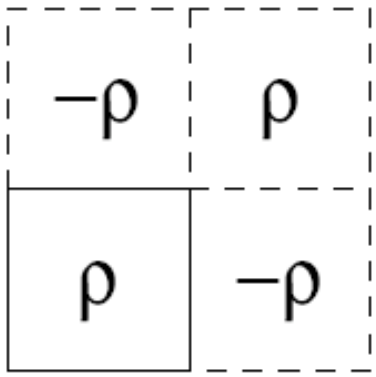
High-Performance Solvers for Potential Theory

$$\varphi(\mathbf{x}) = \int_{\Omega} G(\mathbf{x}-\mathbf{y})\rho(\mathbf{y})d\mathbf{y} \ , \ \mathbf{x} \in \Omega \qquad G(\mathbf{z}) = -\frac{1}{4\pi|\mathbf{z}|}$$

Want multiresolution solvers for gridded data. Applications: AMR-PIC for Vlasov-Poisson, cosmology (particles for collisionless matter, finite-volume method for gas); incompressible flow.

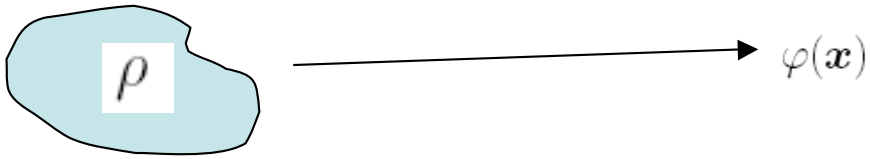
Iterative methods for $\Delta\varphi = \rho$: ~10 flops / grid point between communications steps leads to poor parallel scaling (100s of processors).

Hockney's method for infinite-domain boundary conditions: domain-doubling + FFT. Not adaptive, increases the amount of work by 8x in 3D.



Analysis-Based Poisson Solvers

$$\Delta\varphi = \rho \ , \ \varphi(\boldsymbol{x}) = \int_{\Omega} G(\boldsymbol{x}-\boldsymbol{y})\rho(\boldsymbol{y})d\boldsymbol{y} \ , \ \boldsymbol{x} \in \Omega$$



Real analytic, with rapidly convergent Taylor expansion

Idea: disjoint regions in space are decoupled, modulo analytic functions. Domain decomposition should lead to efficient parallel solvers.

- Multigrid: localizes computation, but not communication.
- Schwarz domain decomposition: still iterative.
- Fast multipole method: localizes computation and communication noniteratively, but cost per point goes up significantly with the number of dimensions.

Method of Local Corrections (Anderson, 1986)

To compute $$\varphi(\mathbf{x}) = \int_{\Omega} G(\mathbf{x}-\mathbf{y})\rho(\mathbf{y})d\mathbf{y} \ , \ \mathbf{x} \in \Omega$$

(1) Solve local problems on overlapping local patches:

$$\varphi(\mathbf{x}) = \int_{\Omega_0^l} G(\mathbf{x}-\mathbf{y})\rho(\mathbf{y})d\mathbf{y} \ , \ \mathbf{x} \in \Omega^l \qquad \bigcup_l \Omega_0^l = \Omega \ , \ \Omega_0^{l'} \bigcap \Omega_0^l = \emptyset$$

(2) Solve a single coarse grid problem to represent the nonlocal coupling:

$$R_{\boldsymbol{i}}^{H,l} = (\Delta^H \phi^l)_{\boldsymbol{i}} \text{ if } \boldsymbol{i}H \in \Omega^l \qquad = 0 \quad \text{otherwise}$$

$$R^H = \sum_l R^{H,l} \qquad \phi^H = G^H * R^H$$

(3) Compute composite solution as combination of local fields and interpolated corrected global field:

$$\phi(\boldsymbol{x}) = \sum_{l:\boldsymbol{x}\in\Omega^l} \phi^l(\boldsymbol{x}) + I(\phi^H - \sum_{l:\boldsymbol{x}\in\Omega^l} \phi^l)(\boldsymbol{x})$$

Field Spreading Using Mehrstellen Operators (Mayo 1982, Anderson 1986)

Let $\phi = G * \rho, supp(\rho) \subset \Omega^l$. Then the error in the field values on the grid satisfies

$$\Delta^H(\phi - \phi^H) = R^{comp}$$

where

$$R_{\boldsymbol{i}}^{comp} = (\Delta^H \phi)_{\boldsymbol{i}} \text{ if } dist(\boldsymbol{i}H, supp(\rho)) > CH$$
$$= 0 \text{ otherwise}$$

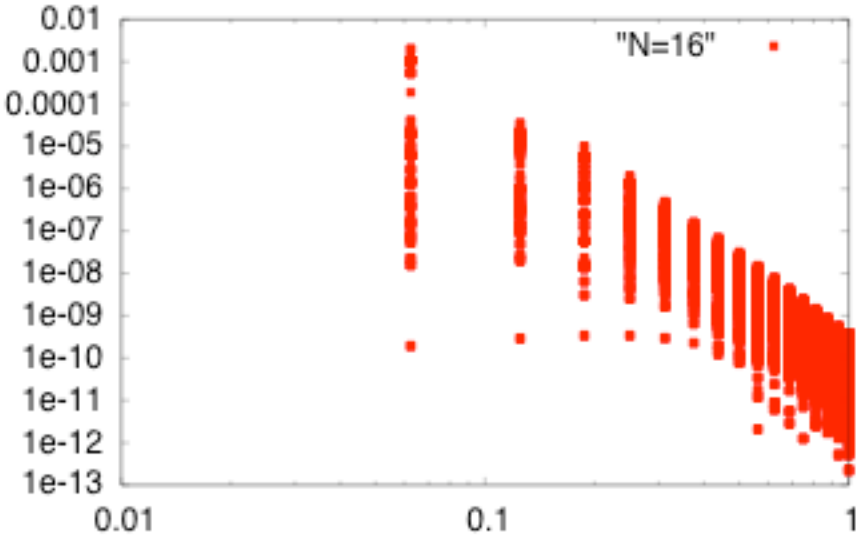
i.e. R^{comp} is the truncation error of Δ^H applied to a harmonic function outside the correction radius.

Mehrstellen Discretizations

19 point: $\Delta_{19}^H \phi = \Delta\phi + \frac{H^2}{12}\Delta\rho + O(H^4)\nabla^6\phi$

27 point: $\Delta_{27}^H \phi = \Delta\phi + \frac{H^2}{12}\Delta\rho + H^4 L^4(\rho) + O(H^6)\nabla^8\phi$

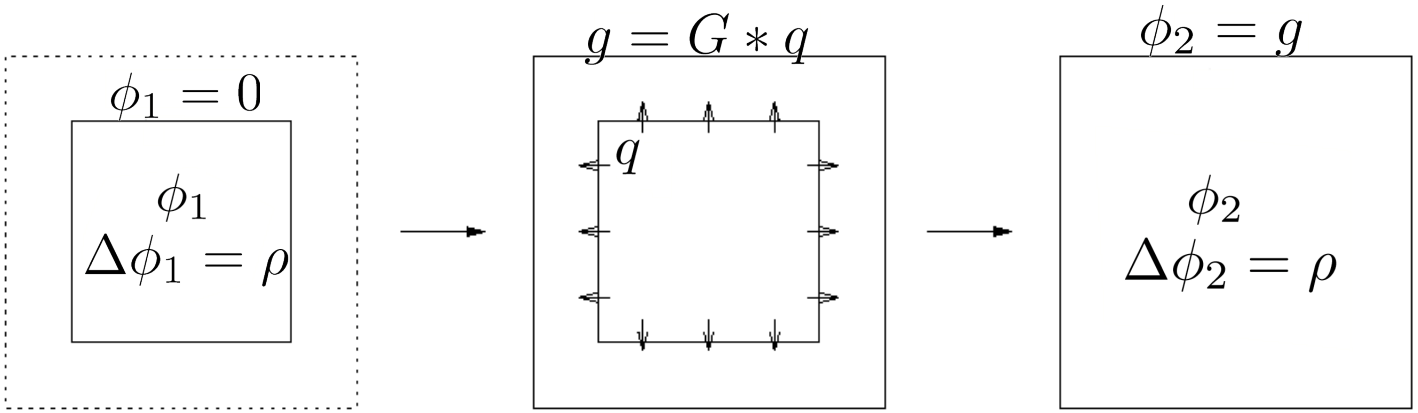
$\Rightarrow R^{comp}$ is a rapidly decreasing function of the distance from the charge. Cutoff distance can be easily tuned to make field spreading arbitrarily accurate.



Scatter plot of $\Delta_{27}^H \phi, H = \frac{1}{16}$ as a function of $||\cdot||_\infty$ distance from support of charge $\rho \equiv 1$ on $[-\frac{1}{2}, \frac{1}{2}]^3$.

Spatial Discretization of Local Solutions

James-Lackner Algorithm for Computing G*ρ (1977)



Solve for ϕ_1 | Compute q, then g | Solve for ϕ_2

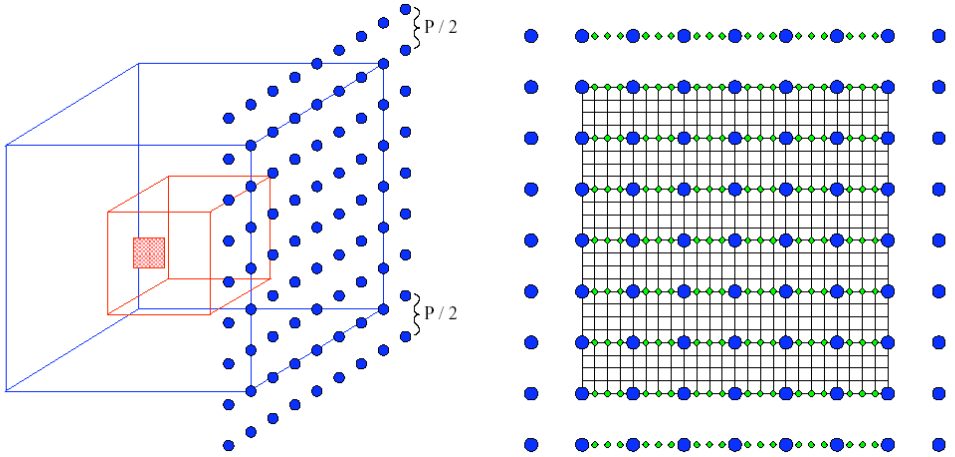
$$q = \frac{\partial \phi}{\partial n} \text{ on } \partial\Omega_1$$

If ρ is piecewise-constant, there is a loss of smoothness leading to a loss of accuracy in the overall MLC algorithm. For this reason, we separate out the monopole components and treat them exactly.

Spatial Discretization of Local Solutions

Fast Multipole Method for the Boundary Potential

In 3D, the direct calculation of the surface-surface potential is too expensive($O(N^{4/3})$). We reduce this to $O(N^{2/3})$ using a simplified multipole expansion. The resulting method is 3X faster than the Hockney domain-doubling method.



Use the 2D multipole expansion on the red patch to evaluate the field on the coarse (blue) grid. The remaining grid points are computed using high-order interpolation.

$$\Phi^{-,2}(\vec{x}) = \sum_{i_0,i_1} \sum_{p_0,p_1} A_{i_0,i_1}^{p_0,p_1,-,2} \times \frac{(-1)^{p_0+p_1}}{p_0!p_1!} \frac{\partial^{p_0+p_1} G}{\partial z_0^{p_0} \partial z_1^{p_1}} (x_0 - i_0 rh, x_1 - i_1 rh, x_2 + s_1 h)$$

Parallel Implementation

Parallel Computation

(1) Local problems are independent, and trivially parallel:

$$\rho = \sum_l \rho^l, supp(\rho^l) \subset \Omega_0^l \qquad \phi^l = G * \rho^l \text{ on } \Omega^l, \Omega^l \supset \Omega_0^l$$

(2) The global solve is a bottleneck, but can itself be parallelized, either by FFT, or applying MLC recursively. It is a much smaller calculation, so there are typically more than enough resources.

$$R^{H,l} = \Delta^H \phi^l \text{ if } \boldsymbol{i}H \in \Omega^l \qquad R^H = \sum_l R^{h,l} \qquad \phi^H = G^H * R^H$$
$$= 0 \text{ otherwise}$$

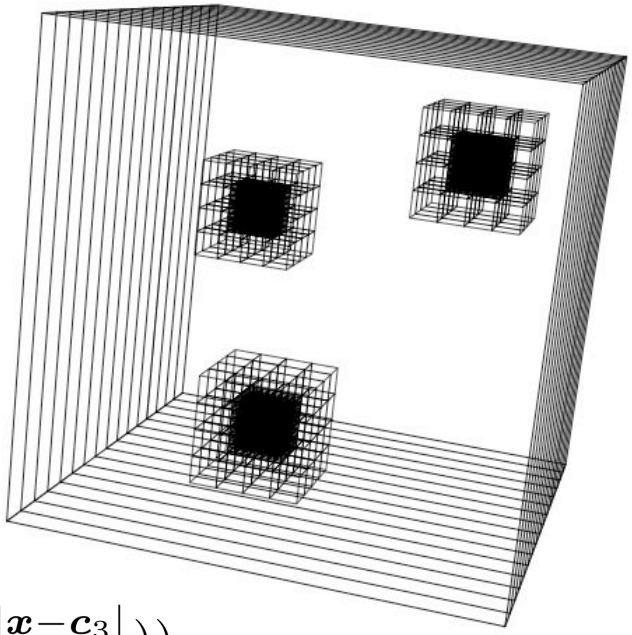
(3) The local interactions / local corrections step is used to compute boundary conditions on patches, which are propagated to the interior by another Dirichlet solve.

$$\phi(\boldsymbol{x}) = \sum_{l:\boldsymbol{x}\in\Omega^l} \phi^l(\boldsymbol{x}) + I(\phi^H - \sum_{l:\boldsymbol{x}\in\Omega^l} \phi^l)(\boldsymbol{x})$$

Parallel Communications Comparable to one multigrid V-cycle: fine-to-coarse between (1) and (2), and coarse-to-fine between (2) and (3), plus an exchange of local fine-fine ghost point data.

Test Problem

- Localized oscillatory charge distribution.
- Two levels of refinement, fixed-size 32^3 patches.
- FFT-based bottom solver, parallelized over 2D slabs.



$$\rho_m^{osc}(r) = \begin{cases} ((r - r^2)\sin(2m\pi r))^2, & \text{if } r < 1; \\ 0, & \text{if } r \geq 1. \end{cases}$$

$$\rho(\boldsymbol{x}) = \frac{1}{R^3}\left(\rho_m^{osc}\left(\frac{|\boldsymbol{x}-\boldsymbol{c}_1|}{R}\right) + \rho_m^{osc}\left(\frac{|\boldsymbol{x}-\boldsymbol{c}_2|}{R}\right) + \rho_m^{osc}\left(\frac{|\boldsymbol{x}-\boldsymbol{c}_3|}{R}\right)\right)$$

Size	three-level example		
N	fine	middle	coarse
2048	50 923 779	6 440 067	2 146 689
4096	405 017 091	21 567 171	16 974 593
8192	3 230 671 875	99 228 483	135 005 697

Results - Accuracy

m	h	$\|\|\epsilon^h_{all}\|\|_\infty$	p	$\|\|\epsilon^h_{fine}\|\|_2$	p	$\|\|\epsilon^h_{all}\|\|_2$	p	λ/h
7	1/2048	2.132×10^{-5}		1.632×10^{-7}		1.738×10^{-7}		7.31
7	1/4096	4.735×10^{-6}	2.17	2.379×10^{-8}	2.78	4.712×10^{-8}	1.88	14.63
7	1/8192	1.130×10^{-6}	2.07	5.720×10^{-9}	2.06	8.419×10^{-9}	2.48	29.26
m	h	$\|\|\epsilon^h_{all}\|\|_\infty$	p	$\|\|\epsilon^h_{fine}\|\|_2$	p	$\|\|\epsilon^h_{all}\|\|_2$	p	λ/h
15	1/2048	2.437×10^{-5}		2.009×10^{-7}		2.357×10^{-7}		3.41
15	1/4096	4.906×10^{-6}	2.31	2.642×10^{-8}	2.93	3.061×10^{-8}	2.95	6.83
15	1/8192	1.157×10^{-6}	2.08	6.648×10^{-9}	1.99	9.737×10^{-9}	1.65	13.65
m	h	$\|\|\epsilon^h_{all}\|\|_\infty$	p	$\|\|\epsilon^h_{fine}\|\|_2$	p	$\|\|\epsilon^h_{all}\|\|_2$	p	λ/h
30	1/2048	5.022×10^{-5}		3.798×10^{-7}		3.848×10^{-7}		1.71
30	1/4096	5.274×10^{-6}	3.25	3.795×10^{-8}	3.32	6.296×10^{-8}	2.61	3.41
30	1/8192	1.542×10^{-6}	1.77	7.593×10^{-9}	2.32	1.270×10^{-8}	2.31	6.83

Three-level convergence results. The wavelength $\lambda = R/(2m) = 1/(40m)$ is a measure of the smallest length scale in the problem.

m	h	$\|\|\epsilon^h_{all}\|\|_\infty$	p	$\|\|\epsilon^h_{fine}\|\|_2$	p	$\|\|\epsilon^h_{all}\|\|_2$	p	λ/h
7	1/2048	4.280×10^{-5}		8.449×10^{-7}		2.608×10^{-6}		7.31
7	1/4096	2.794×10^{-5}	0.62	7.009×10^{-7}	0.27	2.500×10^{-6}	0.06	14.63
7	1/8192	1.971×10^{-5}	0.50	6.713×10^{-7}	0.06	2.521×10^{-6}	−0.01	29.26

Three-level convergence results, without treating the monopole component separately.

Aggregate Performance

	Size	Times for each stage (seconds)							Total	Grind
P	N	InitF	InitM	Crse	BndM	FinM	BndF	FinF	(sec)	(μsec/pt)
16	2048	44.99	12.52	3.51	0.33	0.66	2.64	4.89	69.57	21.86
128	4096	45.51	6.76	10.19	0.15	0.30	4.12	4.75	71.83	22.70
1024	8192	46.01	3.95	13.04	0.15	0.17	4.03	4.78	72.28	22.91

P = number of processors, N = effective grid resolution at the finest level. Grind = proc.-secs. / point

Timings performed on seaborg.nersc.gov.

• Scaled speedup (weak scaling): 95% efficiency up to 1024 processors.

• Aggregate performance: 72 seconds to compute solution on 3 x 10^9 grid points (1024 processors). Comparable to cost / grid point of uniform grid FFT computation, but applied to a locally-refined grid.

Size			Times for each stage (seconds)				Total	Grind
P	N	points	Homo	Normal	FMM	Inhomo	(s)	(μs/pt)
4	256	16 974 593	10.53	0.08	2.23	57.34	70.20	16.54
32	512	135 005 697	13.39	0.87	4.51	22.93	41.72	9.89
256	1024	1 076 890 625	13.65	3.06	10.53	19.26	46.52	11.06

FFT-based infinite-domain solution on uniform grid.

Communications Performance

	Size	Communication in stages (seconds)			Total	% of
P	N	Boundary	Coarse	Residuals	(s)	runtime
16	2048	0.37	0.22	0.08	0.68	0.97 %
128	4096	1.56	0.58	0.14	2.28	3.17 %
1024	8192	1.40	1.77	0.68	3.85	5.32 %

Time spent in MPI communications. Total run times of 69-72 seconds.

- Overall communications costs a few percent of total run time, even up to 1024 processors.
- Most of the non-scaling communication is in the bottom level solver, which uses a parallel FFT.

Future Work

Algorithmic issues

• New version of multilevel algorithm that preserves association of charge distributions with patches.

• Systematic analysis of accuracy using multipole ideas; tunable accuracy.

• Specialized versions for computing gradient fields; extension to diffusion equations, finite-volume discretizations.

• Complex geometries; use as preconditioner for variable-coefficient problems.

Software issues

• Performance tuning, scalability to $\geq 10^5$ processors.

• Robust software components for applications, as opposed to current breadboard implementation.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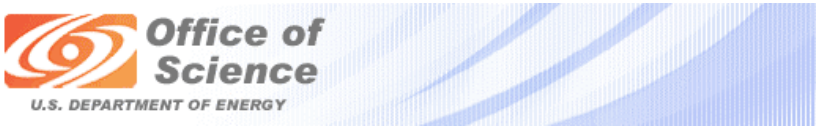
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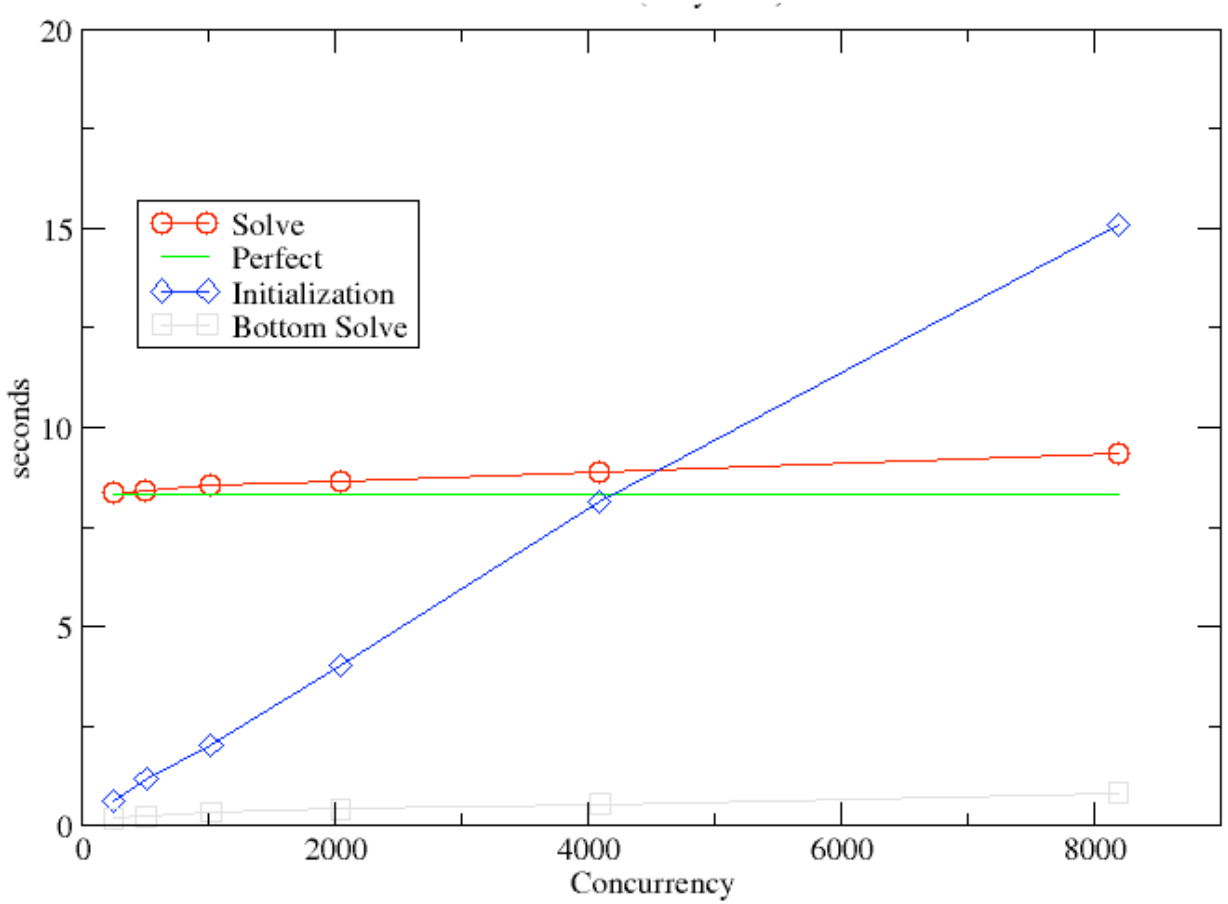
AMRPoisson Solver Weak Scaling



AMR for Petascale Computing

• Preliminary results for hyperbolic PDE indicate scalability of AMR to 10^5 processors.

• Scaling bottleneck for applying AMR to a number of fluid problems (turbulence, self-gravity, kinetic models for charged fluids) is Poisson.

• AMR-MLC has same communications costs, computation / communication ratio as AMR for hyperbolic PDE. Provides possible path forward to petascale for these problems.

Results - Accuracy

	one-grid Mehrstellen				three-level MLC			
m	H	$\|\|\epsilon^H\|\|_\infty / \|\|\phi^{exact}\|\|_\infty$	p	λ/H	h	$\|\|\epsilon^h\|\|_\infty / \|\|\phi^{exact}\|\|_\infty$	p	λ/h
7	1/256	3.52935×10^{-2}		0.91	1/4096	1.05571×10^{-5}		14.63
7	1/512	4.19313×10^{-4}	6.40	1.83	1/8192	2.90449×10^{-6}	1.86	29.26
7	1/1024	1.72642×10^{-5}	4.60	3.66				

	one-grid Mehrstellen				three-level MLC			
m	H	$\|\|\epsilon^H\|\|_\infty / \|\|\phi^{exact}\|\|_\infty$	p	λ/H	h	$\|\|\epsilon^h\|\|_\infty / \|\|\phi^{exact}\|\|_\infty$	p	λ/h
15	1/256	1.01866×10^{-2}		0.43	1/4096	8.38323×10^{-6}		6.83
15	1/512	3.28842×10^{-3}	1.63	0.85	1/8192	3.41383×10^{-6}	1.30	13.65
15	1/1024	1.44633×10^{-4}	4.51	1.71				

	one-grid Mehrstellen				three-level MLC			
m	H	$\|\|\epsilon^H\|\|_\infty / \|\|\phi^{exact}\|\|_\infty$	p	λ/H	h	$\|\|\epsilon^h\|\|_\infty / \|\|\phi^{exact}\|\|_\infty$	p	λ/h
30	1/256	4.55566×10^{-2}		0.21	1/4096	9.27098×10^{-6}		3.41
30	1/512	4.16701×10^{-3}	3.45	0.43	1/8192	2.66318×10^{-6}	1.80	6.83
30	1/1024	9.68717×10^{-4}	2.10	0.85				

Comparison of three-level MLC calculation to uniform-grid Mehrstellen calculations using infinite-domain algorithm.

Spatial Discretization of Local Solutions

FFT Solvers for Volume Potentials

Single-grid Dirichlet solves are done using FFTW fast sine transform. To preserve the strong localization of $\Delta^H \phi^l$, the use of Mehrstellen in the local solves is essential. For example, for the 27-point operator,

$$\phi^{l,h} = \phi^l + h^4 \Psi(x) + O(h^6)$$

where $\Delta\Psi = 0$ away from the support of ρ.

$$\Delta^H \phi^{l,h} = O(h^6) + O(H^6) + O(H^6 h^4)$$