Local Adaptive Refinement on Lattice Gauge Fields

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Local Adaptive Refinement

- The purpose of this talk is to introduce a new numerical method for lattice QCD – Local Adaptive Refinement.
- This method is motivated by the search for improved solvers for the lattice Wilson-Dirac equation $D\psi = \chi$.
- It is strongly motivated by the success of Adaptive Mesh Refinement in computational fluid dynamics, shock hydrodynamics, astrophysics, turbulent flow and combustion.

Adaptive Mesh Refinement in Computational Science

Discussion Based on Martin & Cartwright(1998), Almgren (2011), Guarassi (2015)

- To understand Local Adaptive Refinement it is necessary to understand Adaptive Mesh Refinement (AMR), and why, in its traditional form, it is not suitable for lattice QCD.
- AMR assumes that there is a partial differential equation, which is very difficult to solve, and whose solution involves local inhomogeneity.
- The method works by solving the problem globally at low resolution, and adaptively moves to higher resolution at local regions as the underlying dynamics demand it.

Adaptive Mesh Refinement in Computational Science

When It Works

- Multiscale behavior – Richer detail, more precise on finer grid.
- Local variations in the solution.

Adaptive Mesh Refinement in Computational Science

Partial Differential Equations For Which It Is Used

- Hyperbolic: $u_t + A(u)_x + B(u)_y = 0$ on $D \in \mathcal{R}^2$.
- Poisson: $L\phi = f$ on Ω .

Adaptive Mesh Refinement in Computational Science

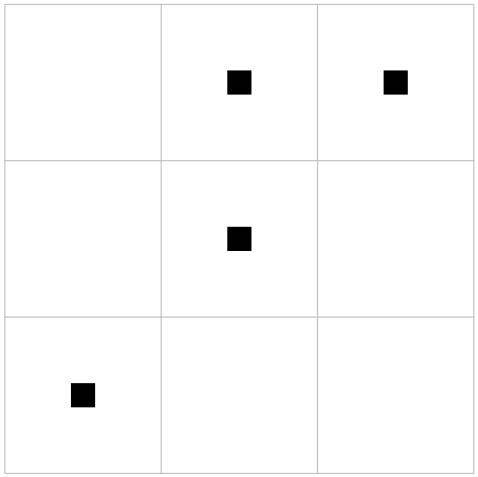
Success Stories

- Shock Hydrodynamics, Berger and Colella (1989), 8X Speedup .
- GPU Fluid Simulation, Wang, Abel, Kaehler (2009), 10X Speedup.
- Parallel AMR Iceberg Production Simulation, X. Zou et. al. (2015), 6X Speedup.

AMR: Block Refinement

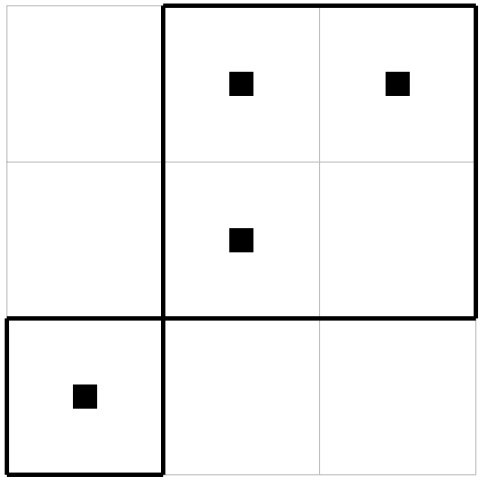
Berger and Oliger (1984)

Cell Refinement



4 Regions Refined

Block Refinement

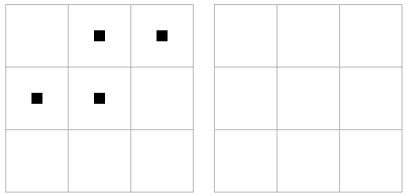


2 Regions Refined

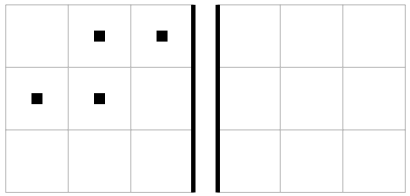
Berger-Rigoutsos Clustering

Berger, Rigoutsos (1991)

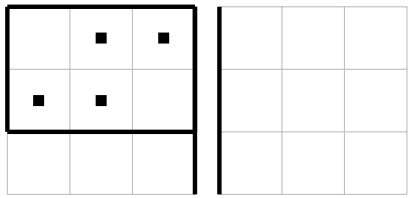
Original Domain



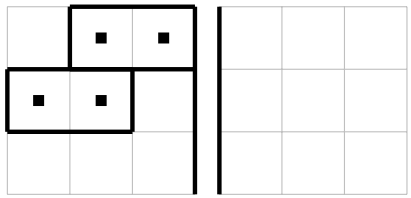
Slicing



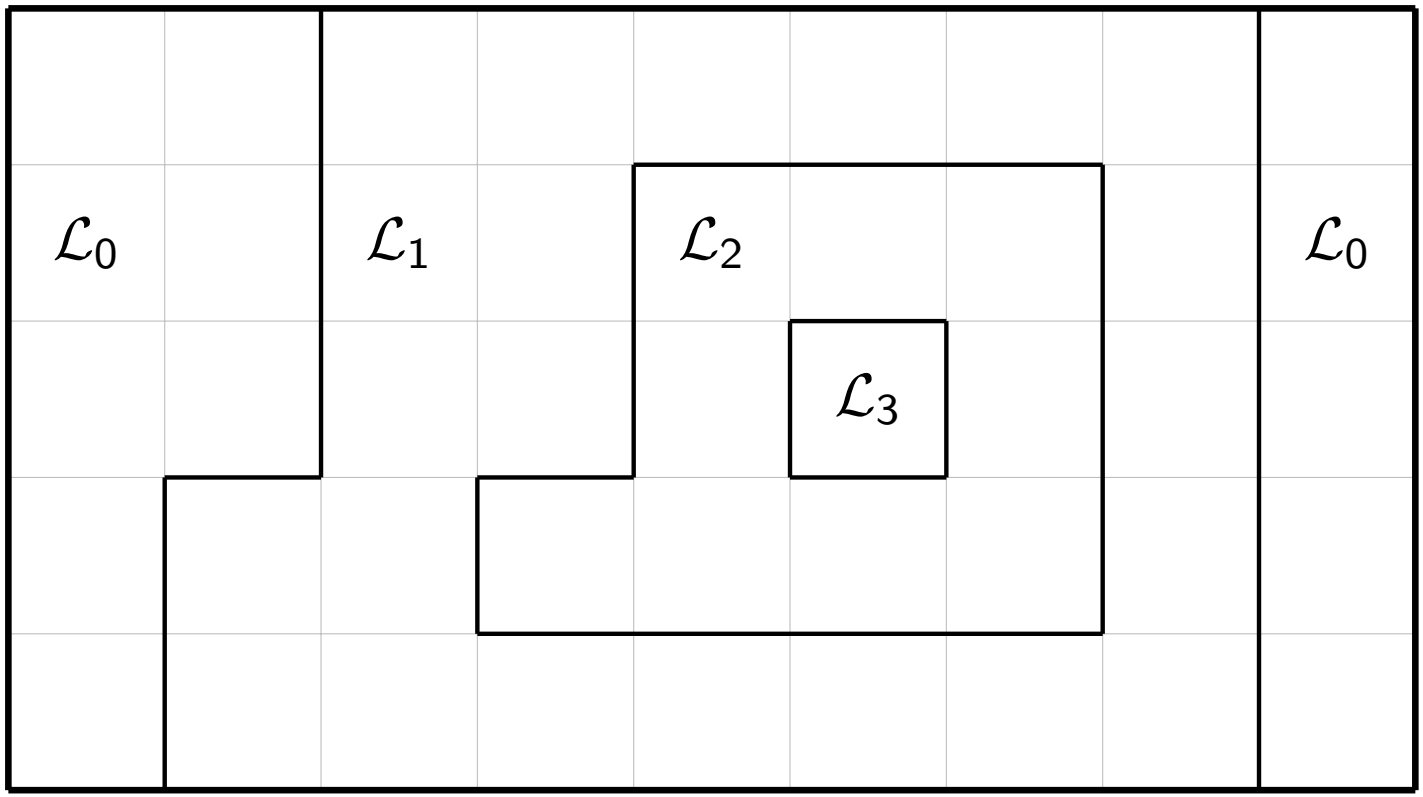
Bounding Box



Splitting



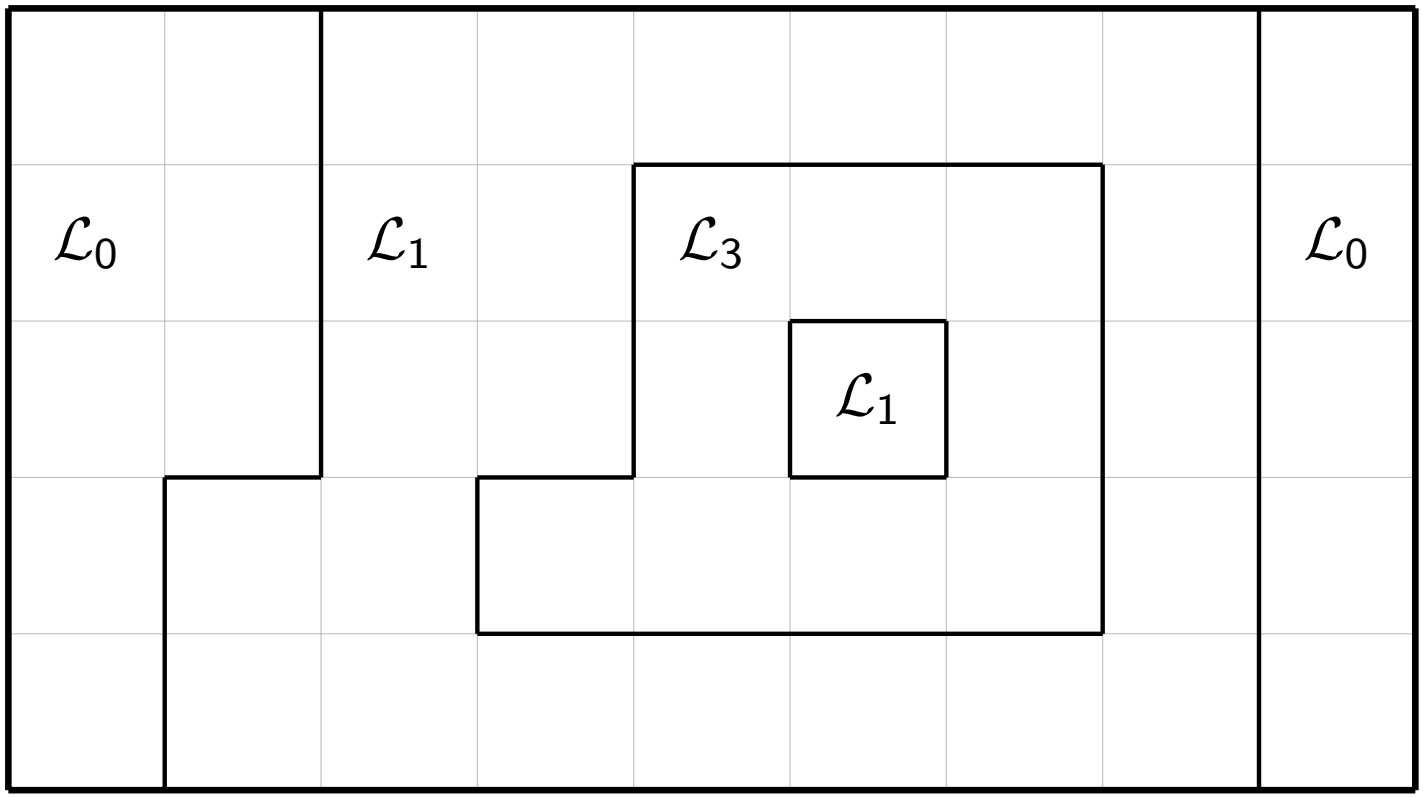
AMR: Intergrid Communications



Proper Nesting

Graphics adapted from Martin, Cartwright (1998)

AMR: Intergrid Communications

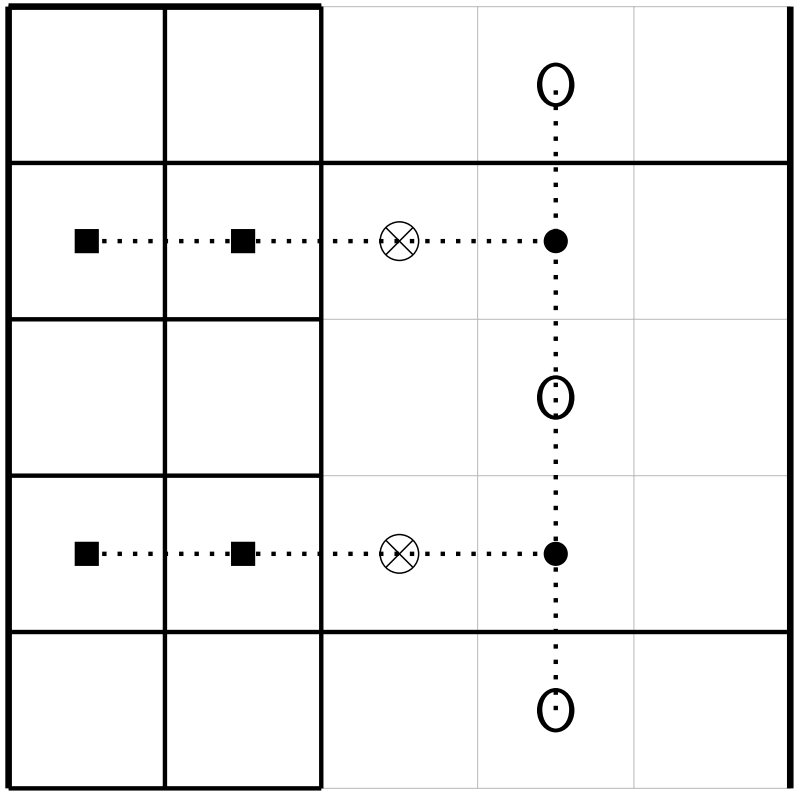


Improper Nesting

Graphics adapted from Martin, Cartwright (1998)

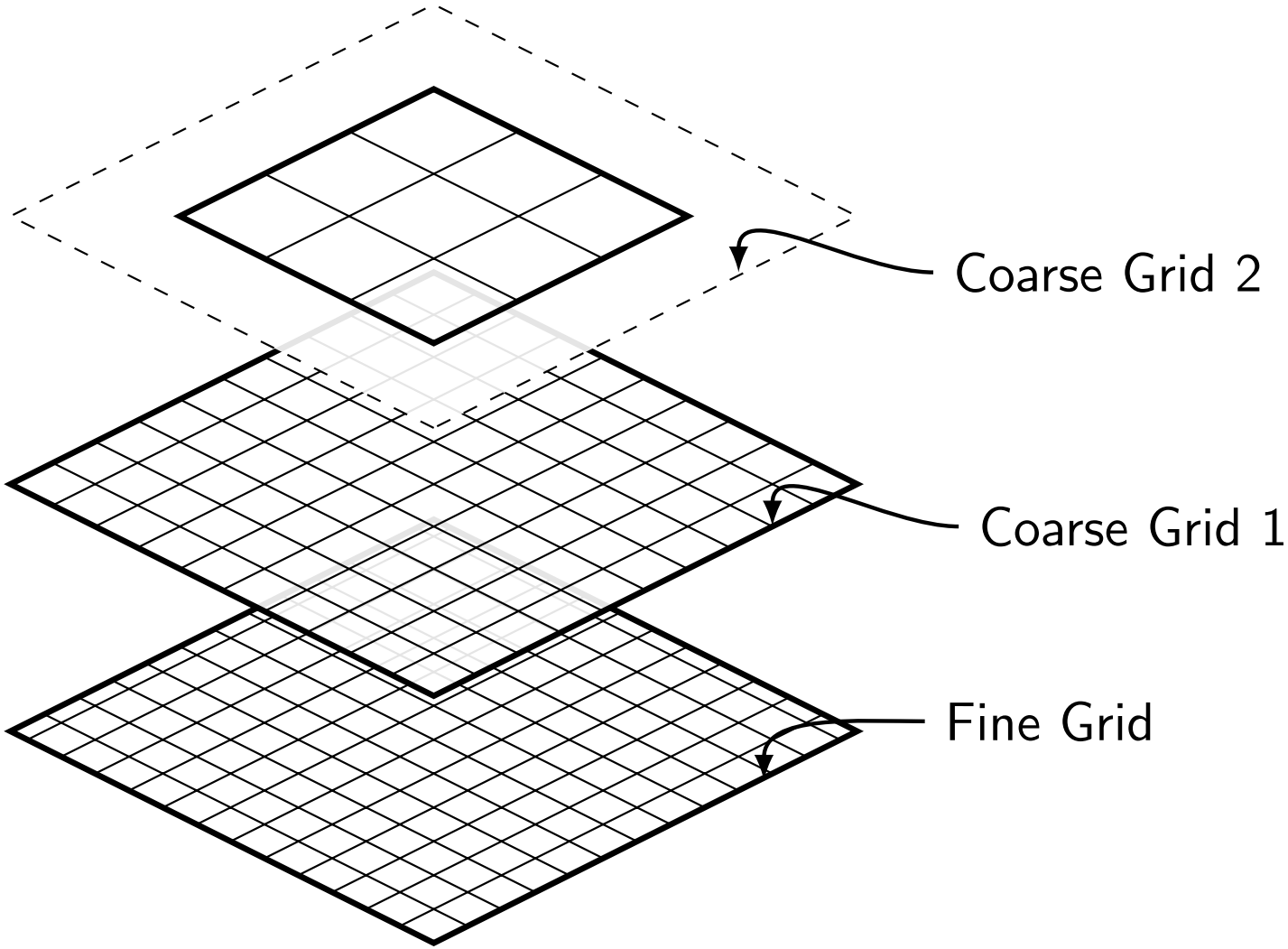
Grid Interfaces

(Flux matching for higher order accuracy)



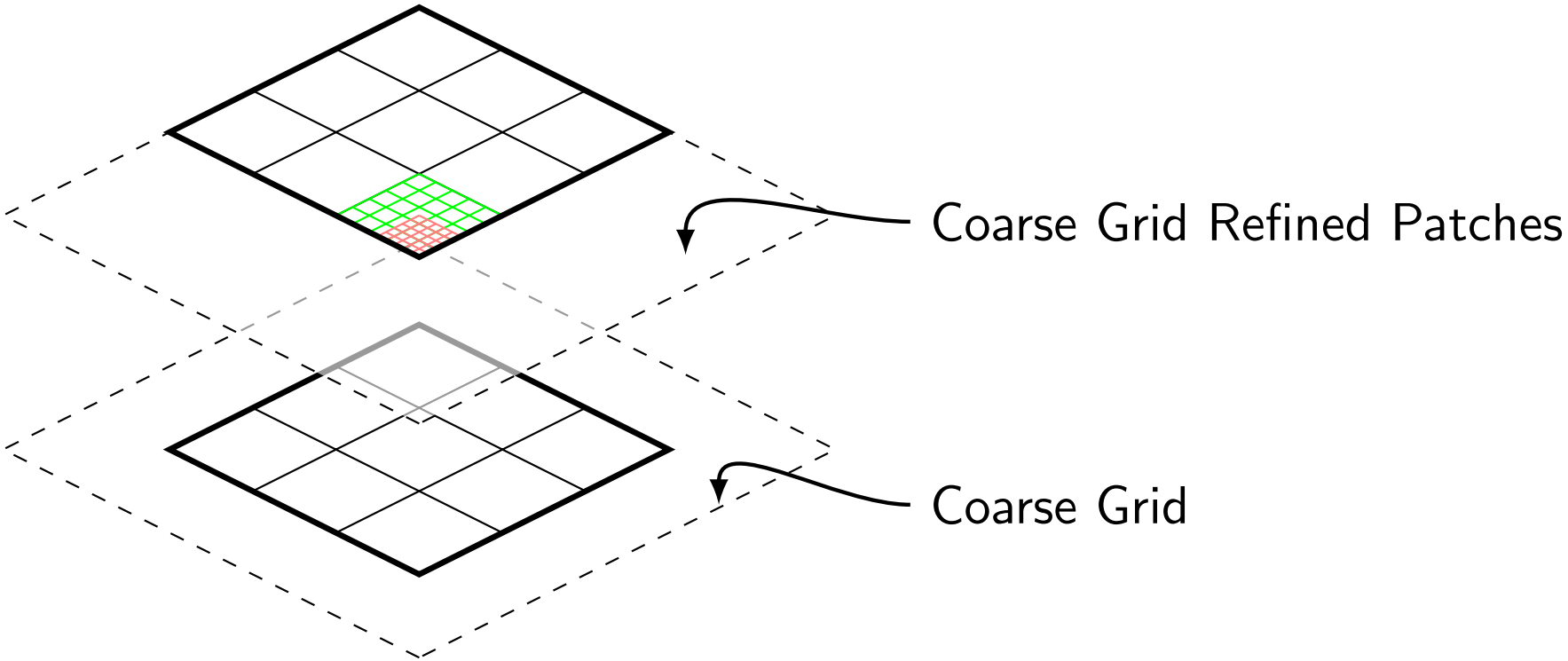
Graphics adapted from P. Colella

Geometric Multigrid Method



Graphics adapted from SWAN model, SWAN Group, TU Delft

AMR Method

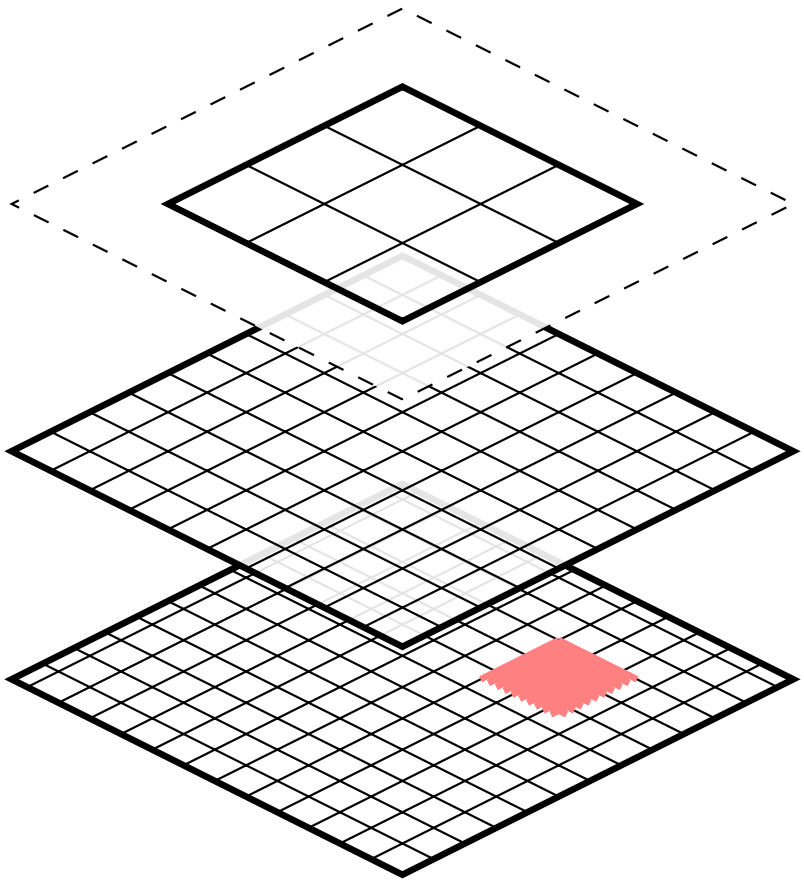


Graphics adapted from SWAN model, SWAN Group, TU Delft

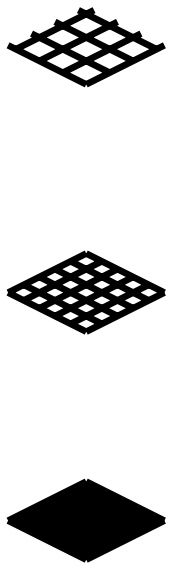
MG With AMR, Separate Cycles

Trottenberg, Oosterlee, Schuller (2001)

Main MG Cycle

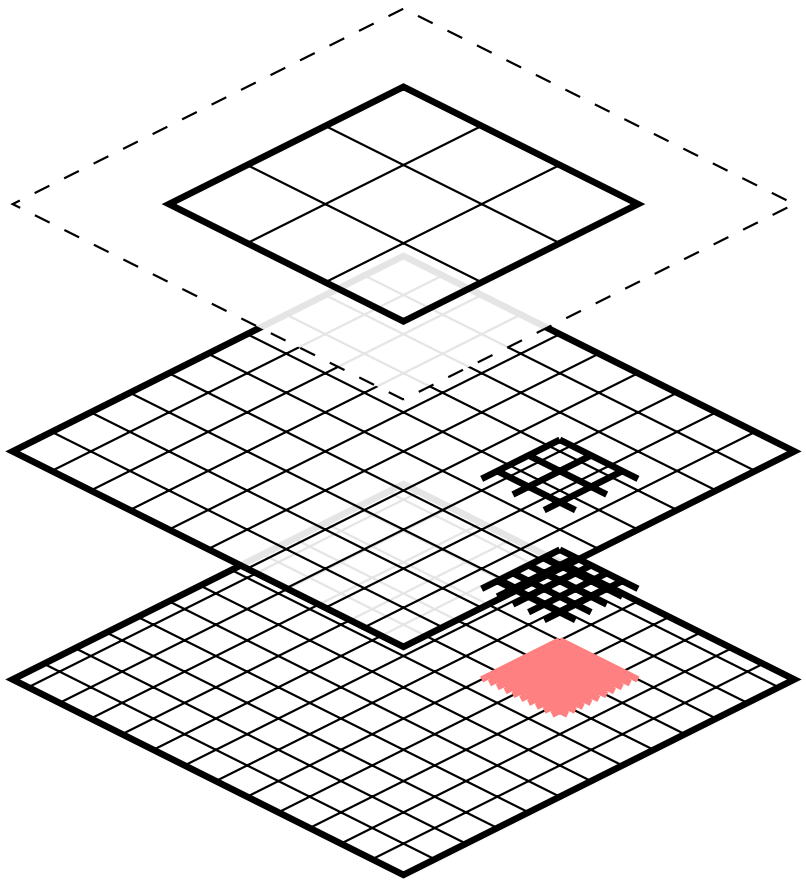


Refined Patch MG Cycle



Graphics adapted from SWAN model, SWAN Group, TU Delft

Multigrid With AMR, Simultaneous MG Cycles



Graphics adapted from SWAN model, SWAN Group, TU Delft

The Problem on the Lattice

- Geometric multigrid methods have never worked well in lattice QCD.
- Traditional AMR, which is highly grid geometry based, may not work well either.
- The success of algebraic multigrid in lattice QCD suggests using an algebraic equivalent of AMR.
- Here, algebraic AMR for lattice QCD will be called Local Adaptive Refinement.

Confusing Nomenclature

- The term "adaptive" may be confusing in this context.
- The term means different things in Algebraic Multigrid and in AMR methods.
- Adaptive Algebraic Multigrid: "adaptive" is an automated procedure to build intergrid operators P and R.
- Local Adaptive Refinement: "adaptive" is an automatic refinement of local variables as a global simulation runs.

Towards Local Adaptive Refinement

The AMG Framework

- The AMG framework of Frommer, Kahl, Kreig, Leder, and Rottmann (2014), uses a block aggregation based approach on a lattice.
- The form of the lattice is $\mathcal{V} = \mathcal{L} \times C \times S$, where $\mathcal{L}$ are points (x,y,z,t) on the lattice, C is color and S is spin.
- The lattice is divided into block aggregates $\mathcal{V}_i = \mathcal{L}_i \times C \times S$
- Form coarser lattices by removing points from $\mathcal{L}_i$. Form finer lattices by adding points to $\mathcal{L}_i$.

Towards Local Adaptive Refinement

The AMG Framework

- Let $\mathcal{V}^B$ be the base lattice, and denote an entire set of lattices by $\mathcal{V}^0, \mathcal{V}^1, ..., \mathcal{V}^B, ..., \mathcal{V}^n$, where $\mathcal{V}^0$ is the finest lattice and $\mathcal{V}^n$ is the coarsest.
- In an MG method with no refinement, $\mathcal{V}^B = \mathcal{V}^0$, and the other lattices are the ones on which coarse grid corrections occur.
- In an MG method with refinement, $\mathcal{V}^B$ lies in between $\mathcal{V}^0$ and $\mathcal{V}^n$.
- Lattices $\mathcal{V}^{B+1}, ..., \mathcal{V}^n$ are used for coarse grid MG corrections. Lattices $\mathcal{V}^0, ..., \mathcal{V}^{B-1}$ are used for local refinement.

Towards Local Adaptive Refinement

The AMG Framework

- Then LAR is like an inverse of AMG, done on local patches.
- As with MG and AMR, block refinement is important. So refine aggregates, rather than individual lattice points.
- As with MG and AMR, proper nesting is important.
- As with MG and AMR, separate or simultaneous cycles can be used.

Towards Local Adaptive Refinement

Integrating The Grid Solutions

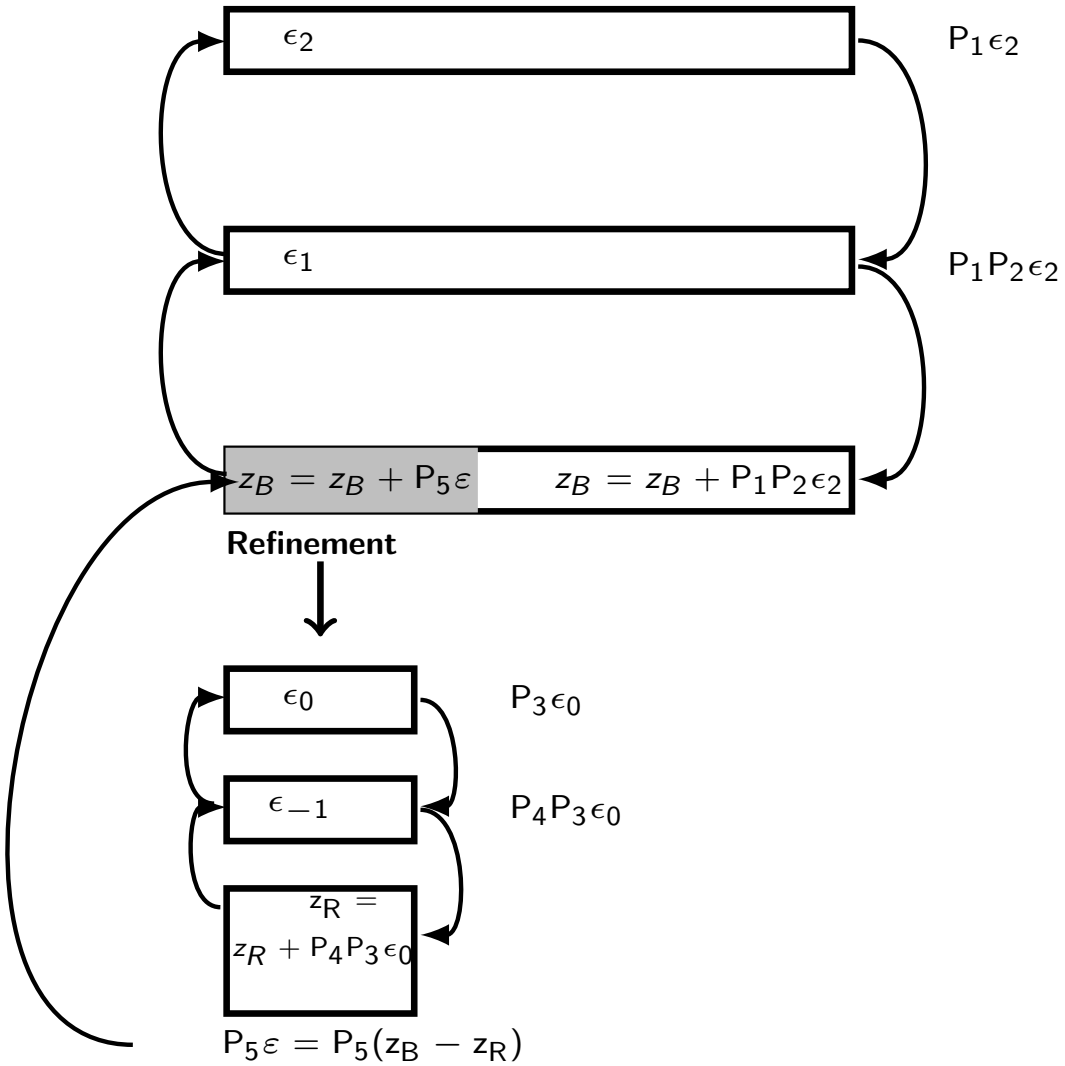
- Unlike MG and AMR, flux matching cannot be used to integrate solutions across boundaries when AMG is used with LAR.
- Suppose that z_B is the solution on the base lattice, and that z_R is the solution on the (localized) refined lattice.
- A naive approach would be to replace z_B with z_R on the refined portion of $\mathcal{V}^B$. But γ_5-Hermiticity might be lost.

Towards Local Adaptive Refinement:

Integrating The Grid Solutions

- Instead, treat the difference between the solution z_B on the base lattice and z_R on the refined lattice as an error term.
- That error term will be $\varepsilon = z_B - z_R$.
- Then interpolate that error term to the base grid, and add it to z_B. The use of P to interpolate ensures γ_5-Hermiticity.

Seamless Integration of Solutions in LAR



Refinement Criterion

Discussion based on Martin, Cartwright (1998)

- Use the error term ϵ computed on each coarse grid during the multigrid cycle.
- Use the local truncation error. Consider $D\psi = \chi$ and lattice levels ordered from finest to coarsest with increasing l. Consider the terms Average$(D^l\psi^l)$ and D^{l-1}Average(ψ^l).
- By the Richardson method, the truncation error is Average$(D^l\psi^l) - D^{l-1}$Average(ψ^l). On unrefined patches of the base lattice, use T^l.

Refinement Criterion

Discussion based on Martin, Cartwright (1998)

- On refined patches, multiply T^l by the refinement ratio (the number of variables on the fine grid patch divided by the number of variables on the coarse grid patch), and average the result over the number of variables on the coarse grid patch.
- Local truncation error is widely used as an error criterion for adaptive refinement.
- It would be prohibitively expensive to calculate at every location on a large lattice.

Parallelization of LAR: Load Balancing

- Multigrid methods may have coarse grid levels with light workloads, leading to idling of processors.
- Refinement methods involve high workloads in local regions, contributing to load balancing problems.
- One can sort refined blocks by size and dynamically allocate them to processors to balance the workload.

Parallelization of LAR: Inter-Process Communications

- Local Adaptive Refinement would involve a large number of simultaneous administrative tasks among several lattice levels.
- Without careful planning, the inter-process communications could become burdensome.
- This will likely be an important programming consideration.

Conclusion

- Adaptive Mesh Refinement has been used successfully in many fields of science and engineering.
- An algebraic version of AMR can be developed in the framework of domain decomposition based algebraic multigrid methods.
- This method is consistent with interpolation and restriction operators that preserve γ_5-Hermiticity.
- Much implementation work remains to be done.

Postscript

- In the question and answer session two conference participants indicated that this method would not work as a solver for a QCD propagator, due to the nature of quantum fields.
- One of these participants suggested that instead the method might be useful in Hybrid Monte Carlo algorithms.
- The other participant suggested an alternative approach based on symplicial gauge field theory methods.
- The author is deeply appreciative of these comments, and is pursuing both lines of investigation.

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