Optimal artificial boundary conditions for three dimensional elliptic random media

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Background

Consider

$$-\nabla \cdot a \nabla u = \nabla \cdot g \tag{E}$$

with

$$\lambda \mathrm{Id} \leq a \leq \mathrm{Id};$$

a symmetric, stationary, unit range, ("i.i.d.");

$$g(x) = \hat{g}(\frac{x}{\ell}), \text{ supp } \hat{g} \subset B_1, \ \ell > 1;$$

u decaying as $x \to \infty$.

Goal: find ∇u in $Q_L = (-L, L)^d$ using information $a|_{Q_{2L}}$ for $L \gg \ell$.

Maxwell: Effective resistance of a composite

A TREATISE

ON

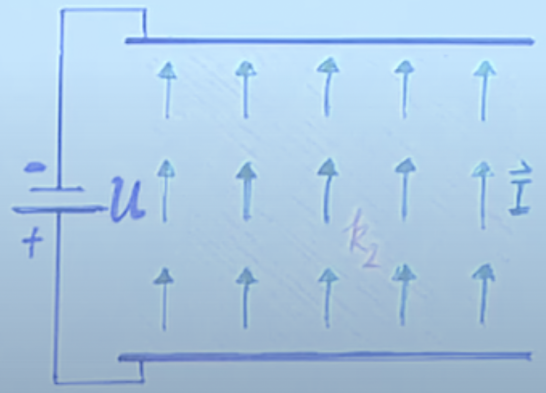
ELECTRICITY AND MAGNETISM

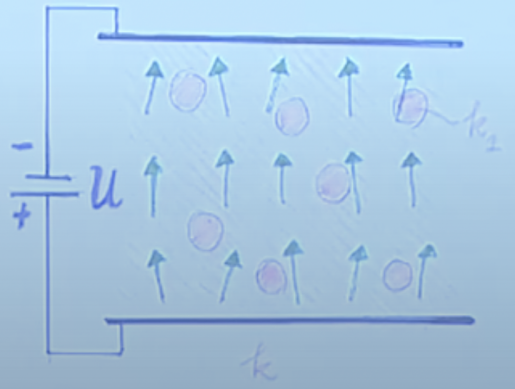
MAXWELL

That the one expression should be equivalent to the other,

$$K = \frac{2k_1 + k_2 + p(k_1 - k_2)}{2k_1 + k_2 - 2p(k_1 - k_2)} k_2. \qquad (17)$$

This, therefore, is the specific resistance of a compound medium consisting of a substance of specific resistance k_2, in which are disseminated small spheres of specific resistance k_1, the ratio of the volume of all the small spheres to that of the whole being p. In order that the action of these spheres may not produce effects depending on their interference, their radii must be small compared with their distances, and therefore p must be a small fraction.





Picture credit to Felix Otto

Background

We have to solve PDEs in a finite box $\Rightarrow$ artificial boundary condition

$$-\nabla \cdot a\nabla \hat{u} = \nabla \cdot g \text{ in } Q_L, \ \hat{u} = ? \text{ on } \partial Q_L.$$

A naive approach: solve for

$$-\nabla \cdot a\nabla u_0 = \nabla \cdot g \text{ in } Q_L, \quad u_0 = 0 \text{ on } \partial Q_L.$$

One can prove $\nabla(u - u_0) = O((\frac{\ell}{L})^d)$. Without any assumption on the structure of a, this is the best we can get.

CLT-Lower Bound

Theorem (Lu, Otto '18)

There exists an ensemble $\langle\cdot\rangle$, which is stationary, of unit-range, such that

$$\Big\langle \Big| \int \eta \nabla u - \langle \int \eta \nabla u | Q_{2L} \rangle \Big|^2 \Big\rangle^{\frac{1}{2}} \geq \frac{1}{C} (\frac{\ell}{L})^d (\frac{1}{L})^{\frac{d}{2}}.$$

Here $\eta > 0$ is compactly supported in an $O(1)$ region and $\int \eta = 1$.

Our goal is to find an algorithm whose error matches the lower bound, which brings us to the framework of stochastic homogenization.

Qualitative Homogenization Theory

The first idea: random media $\Rightarrow$ homogenization

For stationary, ergodic media a, there exists some homogenized coefficient a_h, deterministic and constant in space, and we can consider

$$-\nabla \cdot a \nabla \hat{u} = \nabla \cdot g \text{ in } Q_L, \quad \hat{u} = \tilde{u}_h \text{ on } \partial Q_L,$$

where $\tilde{u}_h$ satisfies

$$-\nabla \cdot a_h \nabla \tilde{u}_h = \nabla \cdot g.$$

Unfortunately, this does not improve the scaling of error in L.

Correctors

The next idea: two-scale expansion.

The corrector ϕ_i on direction e_i is defined (in whole space) as the unique stationary, mean-zero solution of

$$-\nabla \cdot a\nabla(x_i + \phi_i) = 0.$$

We can then look at

$$-\nabla \cdot a\nabla \hat{u} = \nabla \cdot g \text{ in } Q_L, \quad \hat{u} = (1 + \phi_i \partial_i)\tilde{u}_h \text{ on } \partial Q_L.$$

While $(1 + \phi_i \partial_i)\tilde{u}_h$ helps with approximating the gradient, this approach does not improve the scaling of error in L.

What is missing?

The Effective Dipole

- Consider the homogenized equation

$$-\nabla \cdot a_h \nabla \tilde{u}_h = \nabla \cdot g,$$

the solution is given by

$$\tilde{u}_h(x) = \int G_h(x-y) \nabla \cdot g(y) \, \mathrm{d}y.$$

- For $|x| = O(L) \gg |y| = O(\ell)$, we can expand

$$G_h(x-y) = G_h(x) - y_i \partial_i G_h(x) + \text{higher order term}$$

- $$\tilde{u}_h(x) = -\left(\int y_i \nabla \cdot g \, \mathrm{d}y\right) \partial_i G_h(x) + \text{higher order term}$$

- For random media, we replace y_i by $y_i + \phi_i$,

$$u(x) = -\left(\int (y_i + \phi_i) \nabla \cdot g \, \mathrm{d}y\right) \partial_i G_h(x) + \text{higher order term}$$

The Effective Dipole

This extra term motivates us to look at

$$-\nabla \cdot a\nabla \hat{u} = \nabla \cdot g \text{ in } Q_L,$$
$$\hat{u} = (1+\phi_i\partial_i)\Big(\tilde{u}_h - (\int \phi_i \nabla \cdot g)\partial_i G_h\Big) \text{ on } \partial Q_L.$$

This gives an error of $O((\frac{\ell}{L})^d(\frac{1}{L})^{1-})$, and the extra factor $O((\frac{1}{L})^{1-})$ is contributed by the dipole correction. For $d = 2$ this approximation is optimal.

In dimension 3 this algorithm is still $\frac{1}{2}$ order away from being optimal. What else can we do?

Fluxes and Second-Order Correctors

The first-order flux σ_{ijk} is defined as ([Gloria, Neukamm, Otto '14])

$$-\Delta\sigma_{ijk} = \partial_j q_{ik} - \partial_k q_{ij},$$

where $q_i = a(e_i + \nabla\phi_i)$. This enables us to define second-order correctors ψ_{ij}, which satisfy

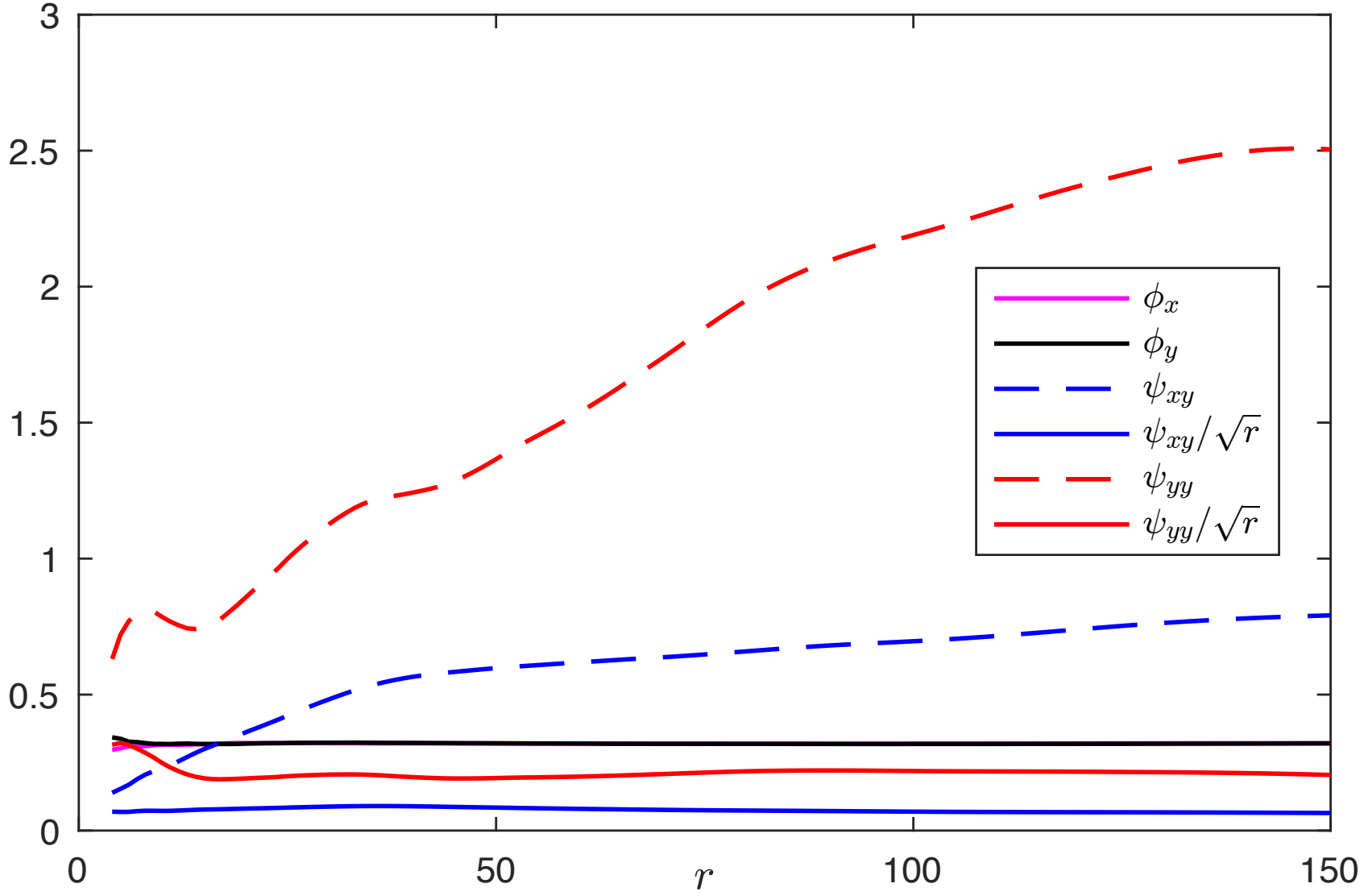
$$-\nabla \cdot a\nabla\psi_{ij} = \nabla \cdot (\phi_i a - \sigma_i)e_j.$$

In 3D the two-scale expansion can be upgraded to ([Bella, Fehrman, Fischer, Otto '17])

$$(1 + \phi_i\partial_i + \psi_{ij}\partial_{ij})\tilde{u}_h.$$

Second-Order Correctors

In 3D ψ has spatial growth like $\sqrt{|x|}$.



Effective Quadrupoles

The solution of homogenized equation $\tilde{u}_h$ should be further corrected by a quadrupole term

$$u_h = \tilde{u}_h - \int (\phi_i \nabla \cdot g) \partial_i G_h + c_{ij} \partial_{ij} G_h,$$

where c_{ij} are some coefficients that can be computed via ϕ, ψ and g [Bella, Giunti, Otto '17].

The solution of

$$-\nabla \cdot a \nabla \hat{u} = \nabla \cdot g \text{ in } Q_L, \quad \hat{u} = (1 + \phi_i \partial_i + \psi_{ij} \partial_{ij}) u_h \text{ on } \partial Q_L,$$

gives the optimal approximation of ∇u.

Optimal Boundary Condition in 3D

Define stochastic norm

$$\|F\|_s := \inf\{M > 0, \langle \exp((\frac{|F|}{M})^s)\rangle \leq 2\}.$$

Theorem (Lu, Otto, W.)

Fix any $\varepsilon > 0$, there exists a random radius r_{**} such that

$$\|r_{**}\|_{\frac{3}{2}-} \lesssim 1.$$

Moreover, for any $R, \ell \in [r_{**}, L]$, we have the following error estimate

$$(\fint_{B_R} |\nabla(\hat{u} - u)|^2)^{\frac{1}{2}} \leq C(\frac{\ell}{L})^d (\frac{r_{**}}{L})^{\frac{3}{2}-\varepsilon}.$$

Here C depends on ellipticity ratio λ, rhs $\hat{g}$ and ε.

Random Radius r_{**}

The radius r_{**} is defined such that (ψ, Ψ) has at most square root growth, where Ψ is the second-order flux:

$$\frac{1}{r^2}\Big(\fint_{B_r} |(\psi,\Psi) - \fint_{B_r}(\psi,\Psi)|^2\Big)^{\frac{1}{2}} \leq (\frac{r_{**}}{r})^{\frac{3}{2}-\varepsilon}, \ \forall r \geq r_{**}.$$

Multipole behavior kicks in when $\ell \geq r_{**}$, since for a_h-harmonic u_h,

$$-\nabla \cdot a\nabla(1 + \phi_i\partial_i + \psi_{ij}\partial_{ij})u_h = -\nabla \cdot (\psi_{ij}a - \Psi_{ij})\nabla\partial_{ij}u_h.$$

For

$$-\nabla \cdot a\nabla\hat{u} = \nabla \cdot g \text{ in } Q_L, \quad \hat{u} = (1 + \phi_i\partial_i + \psi_{ij}\partial_{ij})u_h \text{ on } \partial Q_L,$$

we can control two-scale expansion error by the growth of (ψ, Ψ).

Idealized Algorithm

Algorithm

- *Solve for first-order correctors* ϕ.
- *Determine the homogenized coefficients* a_h.
- *Solve for* $-\nabla \cdot a_h \nabla \tilde{u}_h = \nabla \cdot g$.
- *Solve for first-order flux* σ.
- *Solve for second-order correctors* ψ.
- *Obtain optimal boundary condition* $(1 + \phi_i \partial_i + \psi_{ij} \partial_{ij}) u_h$.
- *Solve for* $\hat{u}$.

In practical computations we have to use a finite domain, therefore we need to find approximations for all these quantities.

Challenges in 3D

In [Lu, Otto '18] a Dirichlet proxy is considered

$$-\nabla \cdot a\nabla(x_i + \phi_i^{(L)}) = 0 \text{ in } Q_{2L},\ \phi_i^{(L)} = 0 \text{ on } \partial Q_{2L}.$$

We hope to prove in 3D

$$\Big(\fint_{Q_L} |\nabla(\phi - \phi^{(L)})|^2\Big)^{\frac{1}{2}} \lesssim L^{-\frac{3}{2}},$$

but we can only prove the error rate to be L^{-1}. Obstacles:

- $\phi^{(L)}$ is not stationary so probabilistic arguments do not apply;
- the effect of boundary layer is unclear.

Massive Approximation

It is well-known [Yurinskii '86] [Gloria, Otto '11] that $\phi_{i,T}$, the solution of the massive equation

$$\frac{1}{T}\phi_{i,T} - \nabla \cdot a\nabla(x_i + \phi_{i,T}) = 0,$$

provides a stationary approximation of ϕ_i. We can further approximate $\phi_{i,T}$ by a "solvable" $\phi_{i,T}^{(L)}$ which satisfies

$$\frac{1}{T}\phi_{i,T}^{(L)} - \nabla \cdot a\nabla(x_i + \phi_{i,T}^{(L)}) = 0 \text{ in } Q_{2L}, \quad \phi_{i,T}^{(L)} = 0 \text{ on } \partial Q_{2L}.$$

Proposition

For any $p < \infty$,

$$\Big(\fint_{Q_L} (\phi_T - \phi_T^{(L)})^2\Big)^{\frac{1}{2}} \lesssim_p (\frac{\sqrt{T}}{L})^p.$$

Pick $\sqrt{T} = L^{1-\varepsilon}$ and we get subalgebraic error.

Massive Approximation

We use the same idea to approximate σ and ψ:

$$\frac{1}{T}\sigma_{ijk,T} - \Delta\sigma_{ijk,T} = \partial_j q_{ik,T} - \partial_k q_{ij,T},$$

$$\frac{1}{T}\psi_{ij,T} - \nabla\cdot a\nabla\psi_{ij,T} = \nabla\cdot((\phi_{i,T}a - \sigma_{i,T})e_j).$$

Proposition

Let r_* be the minimal radius [Armstrong, Smart '14] [Gloria, Neukamm, Otto '14], then for any $\sqrt{T} \geq 1$,

$$\Big\|\Big(\fint_{B_{\sqrt{T}}} |\nabla(\phi_T - \phi)|^2\Big)^{\frac{1}{2}}\Big\|_{2-} \lesssim \sqrt{T}^{-\frac{3}{2}};$$

$$\Big\|I(\ell \geq r_*)\Big(\fint_{B_\ell} |\nabla(\phi_T - \phi)|^2\Big)^{\frac{1}{2}}\Big\|_{2-} \lesssim \sqrt{T}^{-\frac{3}{2}}.$$

$$\Big\|I(\ell \geq r_*)\Big(\fint_{B_\ell} |\nabla(\psi_T - \psi)|^2\Big)^{\frac{1}{2}}\Big\|_{1-} \lesssim \sqrt{T}^{-\frac{1}{2}}.$$

True Algorithm

- Solve for approximate first-order corrector

$$\frac{1}{T}\phi_{i,T}^{(L)} - \nabla \cdot a\nabla\phi_{i,T}^{(L)} = \nabla \cdot ae_i \text{ in } Q_{2L}.$$

- Estimating homogenized coefficients

$$a_h^{(L)}e_i = \fint_{Q_L} q_{i,T}^{(L)}, \text{ for } q_{i,T}^{(L)} = a(e_i + \nabla\phi_{i,T}^{(L)}).$$

- Solve for approximate first-order flux $\sigma_{i,T}^{(L)} = (\sigma_{ijk,T}^{(L)})_{j,k}$

$$\frac{1}{T}\sigma_{ijk,T}^{(L)} - \Delta\sigma_{ijk,T}^{(L)} = \partial_j q_{ik,T}^{(L)} - \partial_k q_{ij,T}^{(L)} \text{ in } Q_{\frac{7}{4}L}.$$

True Algorithm

- Solve for approximate second-order correctors $\psi^{(L)}_{ij,T}$:

$$\frac{1}{T}\psi^{(L)}_{ij,T} - \nabla \cdot a\nabla\psi^{(L)}_{ij,T} = \nabla \cdot (\phi^{(L)}_{i,T}a - \sigma^{(L)}_{i,T})e_j \text{ in } Q_{\frac{3}{2}L}.$$

- Dipole and quadrupole corrections:

$$-\nabla \cdot a^{(L)}_h \nabla \tilde{u}^{(L)}_h = \nabla \cdot g,$$
$$u^{(L)}_h = \tilde{u}^{(L)}_h + (\int \nabla\phi^{(L)}_{i,T} \cdot g)\partial_i G^{(L)}_h + c^{(L)}_{ij,T}\partial_{ij}G^{(L)}_h.$$

- Solve for $u^{(L)}$:

$$\begin{aligned} -\nabla \cdot a\nabla u^{(L)} &= \nabla \cdot g && \text{in } Q_L, \\ u^{(L)} &= (1 + \phi^{(L)}_{i,T}\partial_i + \psi^{(L)}_{ij,T}\partial_{ij})u^{(L)}_h && \text{on } \partial Q_L. \end{aligned}$$

Main Theorem

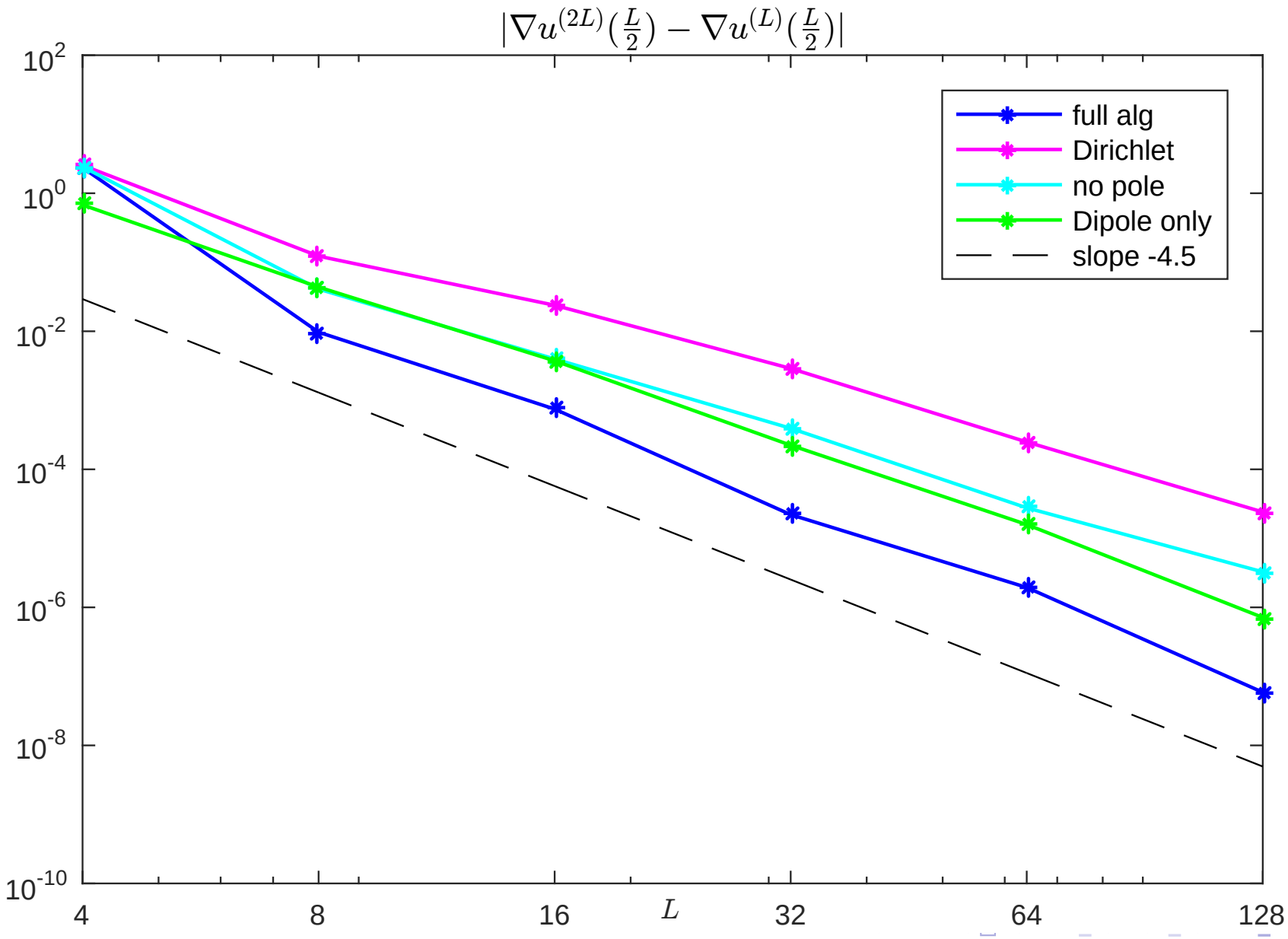
Theorem (Lu, Otto, W.)

Fix $\varepsilon > 0$, the algorithm with $\sqrt{T} = L^{1-\varepsilon}$ produces a function $u^{(L)}$ which only depends on $a|_{Q_{2L}}$, such that conditioning on $\ell \geq r_{**}$, up to an event of probability $\exp(-L^{\frac{\varepsilon}{3}})$, we have

$$\left(\fint_{B_R} |\nabla(u^{(L)} - u)|^2\right)^{\frac{1}{2}} \leq C\left(\frac{\ell}{L}\right)^d \left(\frac{r_{**}}{L}\right)^{\frac{3}{2}-\varepsilon} \text{ for } L \geq R \geq r_{**},$$

Here the constant C depends on λ, ε and $\hat{g}$.

3D Numerical Result



Parabolic Semigroup

For any vector field q_0, we define $S(t)q_0 := v(t)$, which satisfies

$$\partial_t v - \nabla \cdot a\nabla v = 0 \quad \text{for } t > 0, \; v(t=0) = \nabla \cdot q_0.$$

We can then express

$$\phi_i = \int_0^\infty \mathrm{d}t S(t) a e_i, \qquad \text{and} \qquad \phi_{i,T} = \int_0^\infty \mathrm{d}t \exp(-\frac{t}{T}) S(t) a e_i.$$

Proposition (Gloria, Otto '15)

- $$\|(\fint_{B_{\sqrt{T}}} |\nabla S(T) a e|^2)^{\frac{1}{2}}\|_{2-} \lesssim \frac{1}{T}(1 \wedge \frac{1}{\sqrt{T}})^{\frac{d}{2}}.$$
- *$\nabla S(T) a e$ is approximately local on scale $1 \vee \sqrt{T}$.*

Therefore, heuristically in 3D,

$$\nabla(\phi - \phi_T) \lesssim \int_0^\infty \mathrm{d}t (1 - \exp(-\frac{t}{T})) \frac{1}{t} (1 \wedge \frac{1}{\sqrt{t}})^{\frac{3}{2}} \sim \sqrt{T}^{-\frac{3}{2}}.$$

Estimation of ψ

$$\nabla\psi = \int_0^\infty \mathrm{d}t_0 \int_0^\infty \mathrm{d}t_1 \nabla S(t_0)(aS(t_1)ae - \bar{S}(t_1) \times ae)$$
$$- \int_0^\infty \mathrm{d}t_0 \int_0^\infty \mathrm{d}t_1 \int_0^\infty \mathrm{d}t_2 \nabla S(t_0)\bar{S}(t_1) \times a\nabla S(t_2)ae.$$

Proposition

Suppose q_0 is approximately local on scale $r_0 \geq 1$, then:

- $$\|(\fint_{B_{2\sqrt{T}}} |\nabla S(T)q_0|^2)^{\frac{1}{2}}\|_{\frac{2s}{s+2}-} \lesssim \frac{1}{T}\Big(1 \wedge \frac{r_0}{\sqrt{T}}\Big)^{\frac{d}{2}} \|(\fint_{B_{2r_0}} |q_0|^2)^{\frac{1}{2}}\|_s.$$
- *$\nabla S(T)q_0$ is approximately local on scale $r_0 \vee \sqrt{T}$.*

Estimation of r_{**}

We know that $\|r_*\|_3 \lesssim 1$ [Armstrong, Smart '14] [Gloria, Otto '15].

Proposition

For any $R \geq 1$,

$$\|I(R \geq r_*)(\fint_{B_R} |\nabla(\psi, \Psi)|^2)^{\frac{1}{2}}\|_{1-} \lesssim 1;$$

$$\|I(R \geq r_*) \fint_{B_R} \nabla(\psi, \Psi)\|_{1-} \lesssim R^{-\frac{1}{2}}.$$

We use these properties to estimate the probability of $r_{**} \geq R$, which yields the stochastic estimate

$$\|r_{**}\|_{\frac{3}{2}-} \lesssim 1.$$

Future directions:

- Better estimates for Dirichlet proxy of ϕ.
- More general ensembles (for example LSI).
- High contrast/degenerate media.
- Wave propagation in random media.
- Inverse problems.

Thanks for your attention!

References

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