



Rensselaer

## Improving Boundary Derivative Recovery in Elliptic PDEs

David Wells

Rensselaer Polytechnic Institute

In collaboration with:  
J. W. Banks, F. Li

July 13, 2017  
SIAM Annual Meeting

# Outline

- Goals
- A Little on Superconvergence
- $p$ -refinement results in 1D
- Extensions to 2D
- Summary

# Goals

- Efficient numerical methods for elliptic PDEs
- Increased accuracy in (normal) boundary derivatives
- No postprocessing (achieve an energy estimate)
- Order  $n + 1$  data should lead to order  $n + 1$  derivatives

# Goals

(mostly) bilinear elements and order 2 accurate (normal) second derivatives (at isolated points)

## Assumptions

- Linear, constant coefficient elliptic PDEs, Dirichlet (or periodic) boundary conditions
- *Lots of regularity*
- Uniform grid (constant  $\Delta x, \Delta y$ ) of tensor product elements (no triangles)
- Continuous finite element spaces
  - in 1D, degree  $n$  on interior elements, degree  $n + p$  on nonperiodic edge elements
  - in 2D, bilinear on interior elements, degree  $1 \otimes 1 + p$  on nonperiodic edge elements
- Optimal  $L^\infty$  estimates in 1D

$$\left\| \frac{d^m}{dx^m} (u - u^h) \right\|_{L^\infty} \leq C \left\| \frac{d^{m+1}}{dx^{m+1}} u \right\|_{L^\infty} \Delta x^{n+1-m}$$

## Assumptions

- Linear, constant coefficient elliptic PDEs, Dirichlet (or periodic) boundary conditions
- *Lots* of regularity
- Uniform grid (constant  $\Delta x, \Delta y$ ) of tensor product elements (no triangles)
- Continuous finite element spaces
  - in 1D, degree  $n$  on interior elements, degree  $n + p$  on nonperiodic edge elements
  - in 2D, bilinear on interior elements, degree  $1 \otimes 1 + p$  on nonperiodic edge elements
- Optimal  $L^\infty$  estimates in 1D

$$\left\| \frac{d^m}{dx^m} (u - u^h) \right\|_{L^\infty} \leq C \left\| \frac{d^{m+1}}{dx^{m+1}} u \right\|_{L^\infty} \Delta x^{n+1-m}$$

## Assumptions

- Linear, constant coefficient elliptic PDEs, Dirichlet (or periodic) boundary conditions
- *Lots* of regularity
- Uniform grid (constant  $\Delta x$ ,  $\Delta y$ ) of tensor product elements (no triangles)
- Continuous finite element spaces
  - in 1D, degree  $n$  on interior elements, degree  $n + p$  on nonperiodic edge elements
  - in 2D, bilinear on interior elements, degree  $1 \otimes 1 + p$  on nonperiodic edge elements
- Optimal  $L^\infty$  estimates in 1D

$$\left\| \frac{d^m}{dx^m} (u - u^h) \right\|_{L^\infty} \leq C \left\| \frac{d^{m+1}}{dx^{m+1}} u \right\|_{L^\infty} \Delta x^{n+1-m}$$

## Assumptions

- Linear, constant coefficient elliptic PDEs, Dirichlet (or periodic) boundary conditions
- *Lots* of regularity
- Uniform grid (constant  $\Delta x$ ,  $\Delta y$ ) of tensor product elements (no triangles)
- Continuous finite element spaces
  - in 1D, degree  $n$  on interior elements, degree  $n + p$  on nonperiodic edge elements
  - in 2D, bilinear on interior elements, degree  $1 \otimes 1 + p$  on nonperiodic edge elements
- Optimal  $L^\infty$  estimates in 1D

$$\left\| \frac{d^m}{dx^m} (u - u^h) \right\|_{L^\infty} \leq C \left\| \frac{d^{m+1}}{dx^{m+1}} u \right\|_{L^\infty} \Delta x^{n+1-m}$$



## Assumptions

- Linear, constant coefficient elliptic PDEs, Dirichlet (or periodic) boundary conditions
- *Lots* of regularity
- Uniform grid (constant  $\Delta x$ ,  $\Delta y$ ) of tensor product elements (no triangles)
- Continuous finite element spaces
  - in 1D, degree  $n$  on interior elements, degree  $n + p$  on nonperiodic edge elements
  - in 2D, bilinear on interior elements, degree  $1 \otimes 1 + p$  on nonperiodic edge elements
- Optimal  $L^\infty$  estimates in 1D

$$\left\| \frac{d^m}{dx^m} (u - u^h) \right\|_{L^\infty} \leq C \left\| \frac{d^{m+1}}{dx^{m+1}} u \right\|_{L^\infty} \Delta x^{n+1-m}$$

## What's the plan?

- Static  $p$ -refinement: some cells have higher degree polynomial bases
- Global  $h$ -refinement: no mesh adaptivity (yet)
- Not really an  $hp$ -element method, but similar

## What's the plan?

Picking the right type of *p*-refinement improves the boundary derivative convergence rates.

## Superconvergence in 1D

*Classic result:* continuous FE approximation of  $-u_{xx} = f$  with  $V^h =$  piecewise polynomials of degree  $n$  has *zero error* at the knots (cell faces).

*proof:* (Arnold et al, 1972) Consider a knot  $i\Delta x$ :

$$\begin{aligned}|u^h(i\Delta x) - u(i\Delta x)| &= |a(G_{i\Delta x}, u^h - u)| \\ &= |a(G_{i\Delta x} - v^h, u^h - u)| \\ &\leq C \|G_{i\Delta x} - v^h\|_{H^1} \|u^h - u\|_{H^1}\end{aligned}$$

- $G_{i\Delta x}$  is the Green's function centered at  $i\Delta x$
- $G_{i\Delta x}$  is piecewise linear  $\Rightarrow G_{i\Delta x} \in V^h$
- Pick  $G_{i\Delta x} = v^h$ : no knot error!

## Superconvergence in 1D

*Classic result:* continuous FE approximation of  $-u_{xx} = f$  with  $V^h =$  piecewise polynomials of degree  $n$  has *zero error* at the knots (cell faces).

*proof:* (Arnold et al, 1972) Consider a knot  $i\Delta x$ :

$$\begin{aligned}|u^h(i\Delta x) - u(i\Delta x)| &= |a(G_{i\Delta x}, u^h - u)| \\ &= |a(G_{i\Delta x} - v^h, u^h - u)| \\ &\leq C \|G_{i\Delta x} - v^h\|_{H^1} \|u^h - u\|_{H^1}\end{aligned}$$

- $G_{i\Delta x}$  is the Green's function centered at  $i\Delta x$
- $G_{i\Delta x}$  is piecewise linear  $\Rightarrow G_{i\Delta x} \in V^h$
- Pick  $G_{i\Delta x} = v^h$ : no knot error!

## Superconvergence in 1D

*Classic result:* continuous FE approximation of  $-u_{xx} = f$  with  $V^h =$  piecewise polynomials of degree  $n$  has *zero error* at the knots (cell faces).

*proof:* (Arnold et al, 1972) Consider a knot  $i\Delta x$ :

$$\begin{aligned}|u^h(i\Delta x) - u(i\Delta x)| &= |a(G_{i\Delta x}, u^h - u)| \\ &= |a(G_{i\Delta x} - v^h, u^h - u)| \\ &\leq C \|G_{i\Delta x} - v^h\|_{H^1} \|u^h - u\|_{H^1}\end{aligned}$$

- $G_{i\Delta x}$  is the Green's function centered at  $i\Delta x$
- $G_{i\Delta x}$  is piecewise linear  $\Rightarrow G_{i\Delta x} \in V^h$
- Pick  $G_{i\Delta x} = v^h$ : no knot error!

## Superconvergence in 1D

Same idea for  $-u_{xx} + bu_x + cu = f$  (Arnold et al, 1974):

$$\begin{aligned} |u^h(i\Delta x) - u(i\Delta x)| &= |a(G_{i\Delta x}, u^h - u)| \\ &= |a(G_{i\Delta x} - v^h, u^h - u)| \\ &\leq C_1 \|G_{i\Delta x} - v^h\|_{H^1} \|u^h - u\|_{H^1} \\ &\leq C_2 \Delta x^{2k}. \end{aligned}$$

## Superconvergence in 1D

Same idea for  $-u_{xx} + bu_x + cu = f$  (Arnold et al, 1974):

$$\begin{aligned} |u^h(i\Delta x) - u(i\Delta x)| &= |a(G_{i\Delta x}, u^h - u)| \\ &= |a(G_{i\Delta x} - v^h, u^h - u)| \\ &\leq C_1 \|G_{i\Delta x} - v^h\|_{H^1} \|u^h - u\|_{H^1} \\ &\leq C_2 \Delta x^{2k}. \end{aligned}$$



## Superconvergence in 1D

Useful special case for CDR if the last cell consists of piecewise polynomials of degree  $n + p$ ,  $p \geq 1$ , then

$$|u(1 - \Delta x) - u^h(1 - \Delta x)| \leq C\Delta x^{2n+1}$$

*Proof:*

- Same work as before: knot error is bounded by global error times Green's function (interpolation) error
- To the left of  $1 - \Delta x$ : derivatives of the Green's function scale like  $O(\Delta x) \Rightarrow$  we gain an approximation order
- To the right of  $1 - \Delta x$ :  $p \geq 1 \Rightarrow$  we gain (at least) one approximation order

## Superconvergence in 1D

Useful special case for CDR if the last cell consists of piecewise polynomials of degree  $n + p$ ,  $p \geq 1$ , then

$$|u(1 - \Delta x) - u^h(1 - \Delta x)| \leq C\Delta x^{2n+1}$$

*Proof:*

- Same work as before: knot error is bounded by global error times Green's function (interpolation) error
- To the left of  $1 - \Delta x$ : derivatives of the Green's function scale like  $O(\Delta x) \Rightarrow$  we gain an approximation order
- To the right of  $1 - \Delta x$ :  $p \geq 1 \Rightarrow$  we gain (at least) one approximation order

## Improving boundary derivative convergence in 1D

Our first step towards the goal: improving boundary derivative approximation orders for

$$-u_{xx} = f$$

$$\left| \frac{d^m}{dx^m} (u - u^h)(1) \right| \leq C \Delta x^{n+p+1-m}$$

- FE scheme on the boundary cell,  $y^h$ :
  - $y^h(1 - \Delta x) = u^h(1 - \Delta x) = u(1 - \Delta x)$
  - $y^h(1) = u^h(1) = u(1)$
- No knot errors
- Estimates on last cell *don't rely on the rest of the domain* (coupling has zero error)
- Equivalent, discretely, to just doing plain *p*-refinement on the last cell

## Improving boundary derivative convergence in 1D

Our first step towards the goal: improving boundary derivative approximation orders for

$$-u_{xx} = f$$

$$\left| \frac{d^m}{dx^m}(u - u^h)(1) \right| \leq C\Delta x^{n+p+1-m}$$

- FE scheme on the boundary cell,  $y^h$ :
  - $y^h(1 - \Delta x) = u^h(1 - \Delta x) = u(1 - \Delta x)$
  - $y^h(1) = u^h(1) = u(1)$
- No knot errors
- Estimates on last cell *don't rely on the rest of the domain* (coupling has zero error)
- Equivalent, discretely, to just doing plain *p*-refinement on the last cell

## Improving boundary derivative convergence in 1D

Our first step towards the goal: improving boundary derivative approximation orders for

$$-u_{xx} = f$$

$$\left| \frac{d^m}{dx^m}(u - u^h)(1) \right| \leq C\Delta x^{n+p+1-m}$$

- FE scheme on the boundary cell,  $y^h$ :
  - $y^h(1 - \Delta x) = u^h(1 - \Delta x) = u(1 - \Delta x)$
  - $y^h(1) = u^h(1) = u(1)$
- No knot errors
- Estimates on last cell *don't rely on the rest of the domain* (coupling has zero error)
- Equivalent, discretely, to just doing plain  $p$ -refinement on the last cell

## Improving boundary derivative convergence in 1D

Our first step towards the goal: improving boundary derivative approximation orders for

$$-u_{xx} = f$$

$$\left| \frac{d^m}{dx^m}(u - u^h)(1) \right| \leq C\Delta x^{n+p+1-m}$$

- FE scheme on the boundary cell,  $y^h$ :
  - $y^h(1 - \Delta x) = u^h(1 - \Delta x) = u(1 - \Delta x)$
  - $y^h(1) = u^h(1) = u(1)$
- No knot errors
- Estimates on last cell *don't rely on the rest of the domain* (coupling has zero error)
- Equivalent, discretely, to just doing plain *p*-refinement on the last cell

## Improving boundary derivative convergence in 1D

For

$$-u_{xx} + bu_x + cu = f$$

$$\left| \frac{d^m}{dx^m}(u - u^h)(1) \right| \leq C_1 \Delta x^{n+p+1-m} + C_2 \Delta x^{2n-1}$$

- Same as the Laplace equation ( $C_1$ ), but with a nonzero coupling error (saved by better knot estimate,  $C_2 \Delta x^{2n-1}$ )

$m = 2, n = 1, p = 2 \Rightarrow$  linears everywhere, cubics on boundary cells; a second order accurate second derivative on the boundary.

## Improving boundary derivative convergence in 1D

For

$$-u_{xx} + bu_x + cu = f$$

$$\left| \frac{d^m}{dx^m}(u - u^h)(1) \right| \leq C_1 \Delta x^{n+p+1-m} + C_2 \Delta x^{2n-1}$$

- Same as the Laplace equation ( $C_1$ ), but with a nonzero coupling error (saved by better knot estimate,  $C_2 \Delta x^{2n-1}$ )

$m = 2, n = 1, p = 2 \Rightarrow$  linears everywhere, cubics on boundary cells; a second order accurate second derivative on the boundary.



## Improving boundary derivative convergence in 1D

For

$$-u_{xx} + bu_x + cu = f$$

$$\left| \frac{d^m}{dx^m}(u - u^h)(1) \right| \leq C_1 \Delta x^{n+p+1-m} + C_2 \Delta x^{2n-1}$$

- Same as the Laplace equation ( $C_1$ ), but with a nonzero coupling error (saved by better knot estimate,  $C_2 \Delta x^{2n-1}$ )

$m = 2, n = 1, p = 2 \Rightarrow$  linears everywhere, cubics on boundary cells; a second order accurate second derivative on the boundary.

## Improving boundary derivative convergence in 1D

For

$$-u_{xx} + bu_x + cu = f$$

$$\left| \frac{d^m}{dx^m}(u - u^h)(1) \right| \leq C_1 \Delta x^{n+p+1-m} + C_2 \Delta x^{2n-1}$$

- Same as the Laplace equation ( $C_1$ ), but with a nonzero coupling error (saved by better knot estimate,  $C_2 \Delta x^{2n-1}$ )

$m = 2, n = 1, p = 2 \Rightarrow$  linears everywhere, cubics on boundary cells; a second order accurate second derivative on the boundary.

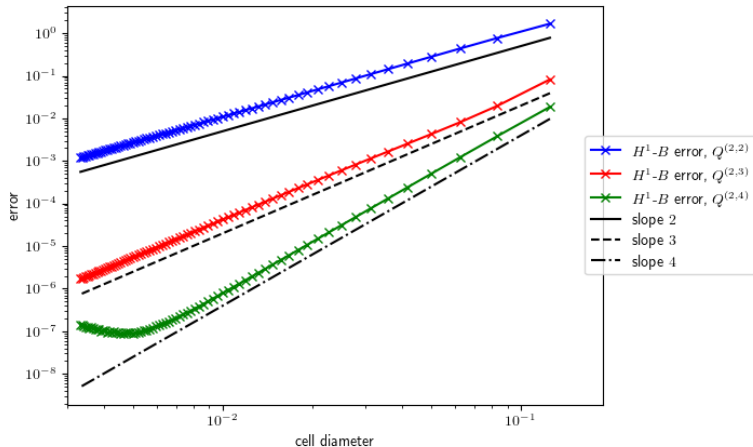
## Numerical Results

Domain of  $[0, 1]$ , with manufactured solution

$$u = \sin(10x)$$

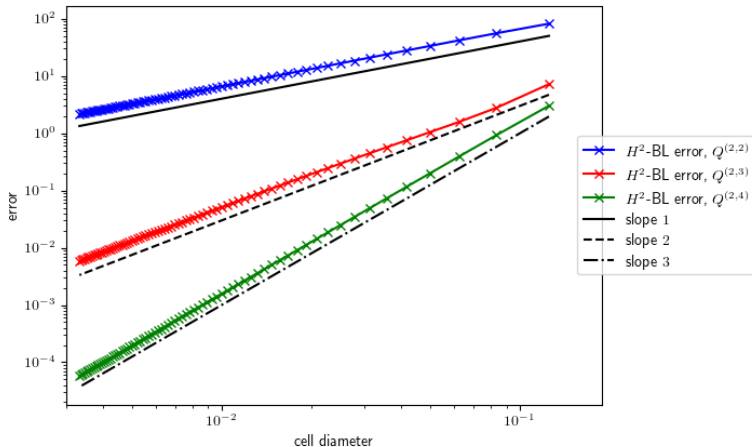
- Use `deal.II`'s *hp*-finite element support
- Bulk order 2, boundary orders 2, 3, and 4
- CDR equation
- Solve with GMRES

## Numerical Results



Convergence rates for the *p*-refinement scheme of the first derivative on the boundary. We hit roundoff error near the end.

## Numerical Results



Convergence rates for the *p*-refinement scheme of the second derivative on the boundary.

## Extensions to 2D

With periodic boundary conditions in  $x$  and Dirichlet boundary conditions in  $y$ ,  
 $\sqrt{-1} = l$ :

$$-\Delta u + \vec{b} \cdot \nabla u + cu = f \Rightarrow -\hat{u}_{yy} + b_2 \hat{u}_y + (k^2 + lkb_1 + c)\hat{u} = \hat{f}_k$$

If we can handle the Fourier transform somehow then we are set.

## Extensions to 2D

Linear elements in  $x \Rightarrow$  centered differences in  $x$ :

$$D^0 U_i = \frac{U_{i+1} - U_{i-1}}{2\Delta x}$$
$$D^+ D^- U_i = \frac{U_{i+1} - 2U_i + U_{i-1}}{\Delta x^2}$$

## Extensions to 2D

- Discrete in  $x$ , continuous in  $y$
- The solution in  $x$  is a superposition of grid eigenfunctions  $\exp(ikx_j) \Rightarrow$  calculate errors for each  $k$  and sum them up via inverse discrete Fourier transform

$$u(x_j, y) \approx \sum_{k=-N/2}^{N/2} \exp(ikx_j) Y_k(y)$$

$$-Y_k''(y) + b_2 Y_k'(y) + \left( \frac{4 \sin^2(k\Delta x/2)}{\Delta x^2} + \frac{b_1 \sin(k\Delta x)}{\Delta x} + \frac{4 + 2 \cos(k\Delta x)}{6} c \right) Y_k(y) = F_k(y).$$



## Extensions to 2D

- Discrete in  $x$ , continuous in  $y$
- The solution in  $x$  is a superposition of grid eigenfunctions  $\exp(ikx_i) \Rightarrow$  calculate errors for each  $k$  and sum them up via inverse discrete Fourier transform

$$u(x_i, y) \approx \sum_{k=-N/2}^{N/2} \exp(ikx_i) Y_k(y)$$

$$-Y_k''(y) + b_2 Y_k'(y) + \left( \frac{4 \sin^2(k\Delta x/2)}{\Delta x^2} + \frac{b_1 / \sin(k\Delta x)}{\Delta x} + \frac{4 + 2 \cos(k\Delta x)}{6} c \right) Y_k(y) = F_k(y).$$

## Extensions to 2D

- Discrete in  $x$ , continuous in  $y$
- The solution in  $x$  is a superposition of grid eigenfunctions  $\exp(ikx_i) \Rightarrow$  calculate errors for each  $k$  and sum them up via inverse discrete Fourier transform

$$u(x_i, y) \approx \sum_{k=-N/2}^{N/2} \exp(ikx_i) Y_k(y)$$

$$-Y_k''(y) + b_2 Y_k'(y) + \left( \frac{4 \sin^2(k\Delta x/2)}{\Delta x^2} + \frac{b_1 \sin(k\Delta x)}{\Delta x} + \frac{4 + 2 \cos(k\Delta x)}{6} c \right) Y_k(y) = F_k(y).$$

## Extensions to 2D

$$\left| \frac{d^m}{dx^m} \left( u(x, y) - u^h(x, y) \right) \right|_{(\delta_i, \delta_{N^*})} \leq C_1 \Delta x^2 + C_2 \Delta y^{2+p-m}$$

where  $N^* = 0$  or  $N^* = N$ .

*proof outline:*

- $x$ -discretization is  $O(\Delta x^2)$  from the Fourier solution; higher-frequency modes have a small contribution (regularity assumption)
- Derivatives of the Green's function scale like  $O(k^{m-1})$ : controlled by the decay of the Fourier coefficients (regularity assumption)
- Sums in the inverse Fourier transform converge with no loss in approximation order

*Important:* this only proves convergence at *knots*.

## Numerical Results

Manufactured solution with  $\vec{b} = (1, 1)$  and  $c = 2$ :

$$u(x, y) = (y^3 + \exp(-y^2) + \sin(4.5y^2) + \sin(20y))(20 \cos(4\pi x) + 0.1 \sin(20\pi x) - 80 \sin(6\pi x))$$

$H^1$ -B error defined as

$$\max_{i,j} \left| (\nabla u^h \cdot \vec{n} - \nabla u \cdot \vec{n})(\delta_i, \delta_j) : (\delta_i, \delta_j) \in \partial\Omega^h \right|$$

and  $H^2$ -B error defined as

$$\max_{i,j} \left| (\vec{n}^T \Delta u^h \cdot \vec{n} - \vec{n}^T \Delta u \cdot \vec{n})(\delta_i, \delta_j) : (\delta_i, \delta_j) \in \partial\Omega^h \right|.$$

## Numerical Results

Manufactured solution with  $\vec{b} = (1, 1)$  and  $c = 2$ :

$$u(x, y) = (y^3 + \exp(-y^2) + \sin(4.5y^2) + \sin(20y))(20 \cos(4\pi x) + 0.1 \sin(20\pi x) - 80 \sin(6\pi x))$$

$H^1$ - $B$  error defined as

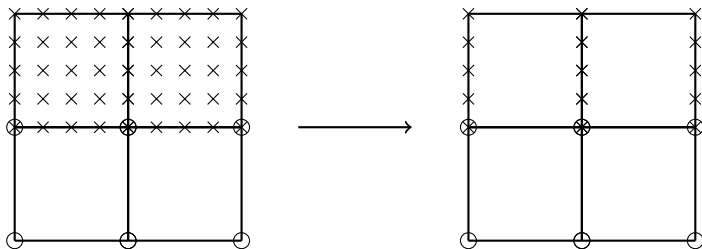
$$\max_{i,j} \left| (\nabla u^h \cdot \vec{n} - \nabla u \cdot \vec{n})(\delta_i, \delta_j) : (\delta_i, \delta_j) \in \partial\Omega^h \right|$$

and  $H^2$ - $B$  error defined as

$$\max_{i,j} \left| (\vec{n}^T \Delta u^h \cdot \vec{n} - \vec{n}^T \Delta u \cdot \vec{n})(\delta_i, \delta_j) : (\delta_i, \delta_j) \in \partial\Omega^h \right|.$$

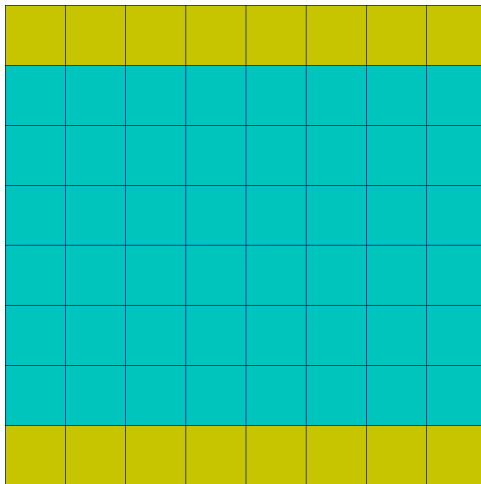
## Numerical Results

Elimination of nonnormal  $p$ -refinement:



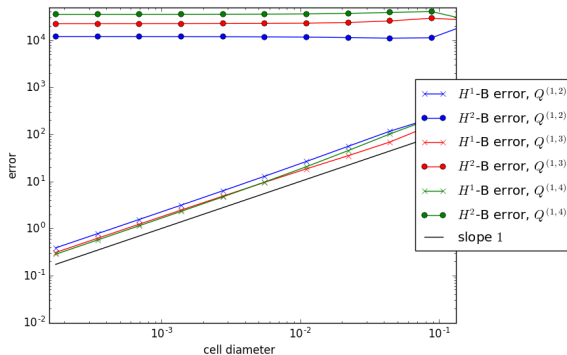
Depiction of normal  $p$ -refinement scheme, with elimination of extra DoFs. Linear DoFs are circles, quartic are crosses.

## Numerical Results



Depiction of the square grid with bulk cells in cyan and  $p$ -refined cells in yellow.

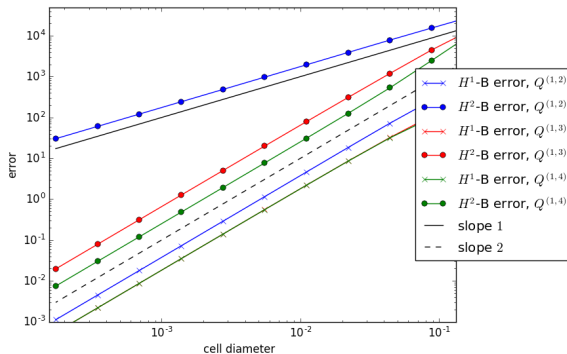
## Numerical Results



Convergence rates with anisotropic  $p$ -refinement. We do not recover any higher order accurate derivatives.

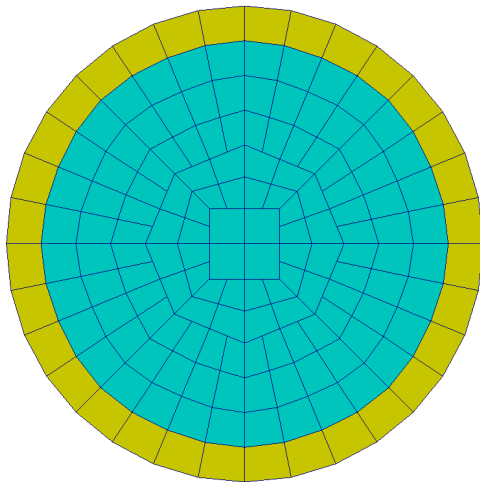


## Numerical Results



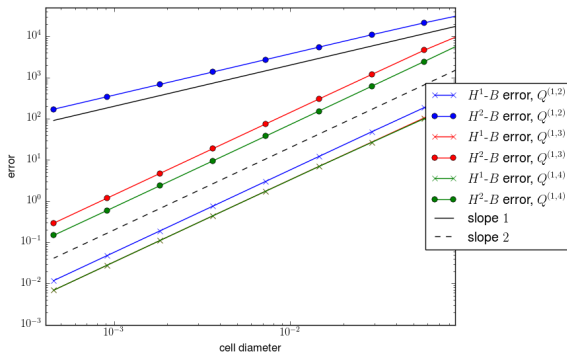
Convergence rates with isotropic *p*-refinement. The 1D theory applies at the knots.

## Numerical Results



A circular grid with a geometry described near the boundary in polar coordinates, in the middle with Cartesian coordinates, and a transfinite interpolation in-between.

## Numerical Results



Rates of convergence for the circular grid.

## Summary and Outlook

- $p$ -refinement error estimates involve a coupling term and a local term
- We can achieve higher-order derivative approximation at isolated points
- Future work: escape the Fourier framework, higher-order bulk elements, better tools for describing arbitrary geometries

Thank You!