A fourth order finite difference method for solving elliptic interface problems with the FFT acceleration

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Conference on Fast Direct Solvers

October 24, 2021

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Funding support

NSF DMS-1812930

NSF DMS-2110914

Outline

1. **Elliptic interface problem**

2. **Poisson boundary value problem (BVP)**
   - 4^{th} - 8^{th} order for 2D & 3D cubic domains
   - FFT for any boundary condition

3. **Poisson interface problem**
   - Fourth order accuracy for curved interfaces
   - FFT for both interface and boundary

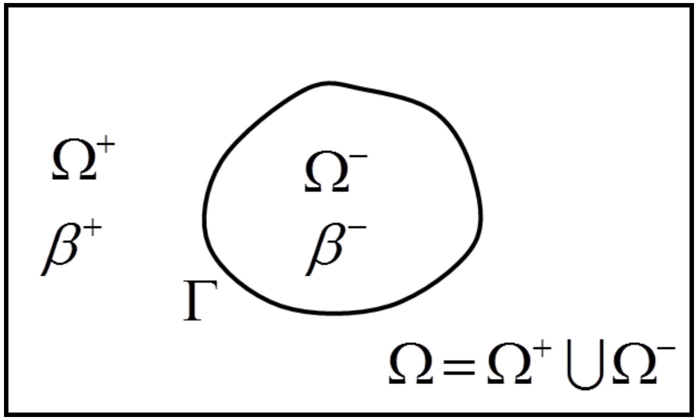
4. **Summary**

1. Elliptic interface problem

Poisson's equation over a rectangular domain

$$\begin{aligned} -\nabla \cdot (\beta \nabla u) &= f(\vec{x}), \qquad \vec{x} \in \Omega \\ u &= g(\vec{x}), \qquad \vec{x} \in \partial\Omega \end{aligned} \qquad (1)$$

where $\beta = \begin{cases} \beta^+, & \vec{x} \in \Omega^+ \\ \beta^-, & \vec{x} \in \Omega^- \end{cases}$

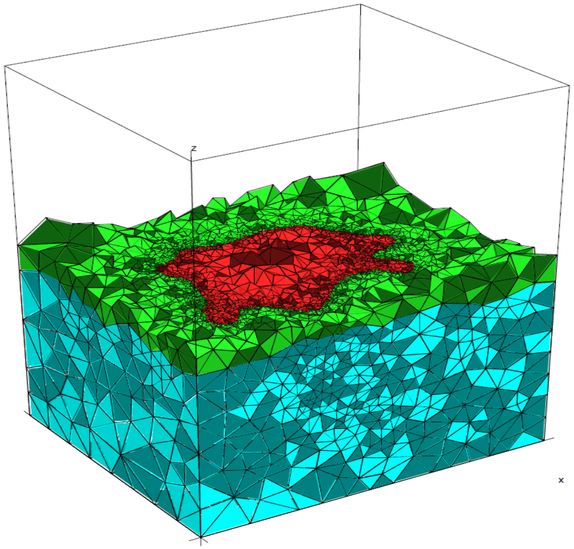


- **General jump conditions**

$$\begin{aligned} [u] &:= u^+ - u^- = \phi(\vec{x}) \\ [\beta u_n] &:= \beta^+ \nabla u^+ \cdot \vec{n} - \beta^- \nabla u^- \cdot \vec{n} = \psi(\vec{x}) \end{aligned} \qquad (2)$$

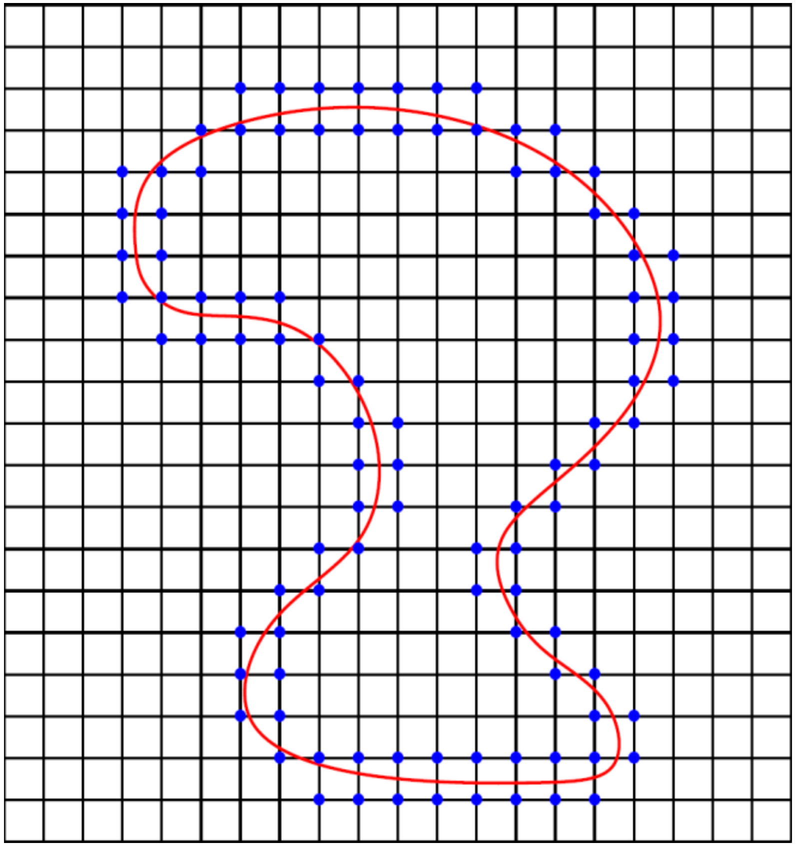
Body-fitted meshes

- **Finite element methods (FEMs)**
  - Pioneer studies *(Babuska 1970; Chen, Zou 1998)*
  - Immersed FEM (IFEM) *(Ewing, Li, Lin, Lin 1999)*
  - Extended FEM (XFEM) *(Ji, Dolbow 2004)*
  - Discontinuous Galerkin *(Huynh et. 2013)*
  - Weak Galerkin *(Mu et. 2013)*
  - …
- **Finite volume methods**
- **Integral equation methods**



Cartesian grid methods

- Immersed boundary method *(Peskin 1977)*
- Immersed interface method (IIM) *(LeVeque, Li, 1994)*
- Ghost fluid method *(Fedkiw, Osher, Liu 2000)*
- Matched interface and boundary (MIB) *(Zhou, Zhao, Wei 2006)*
- …



Fast Poisson solvers for interface problems

- Geometric multigrid solver O(N)
  - IIM *(Adams, Li, 2004)*
  - Piecewise-polynomial interface method *(Chen, Strang, 2008)*
  - Ghost fluid method *(Coco, Russo, 2018)*
  - Virtual node method *(Bedrossian, et. 2010)*

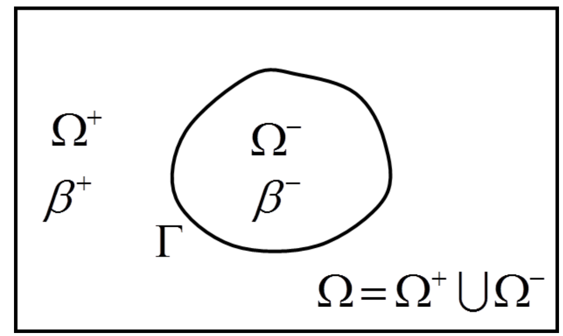
- Fast Fourier transform (FFT) O(N logN)
  - Augmented IIM *(Li 1998)*
  - Explicit Jump IIM *(Wiegmann, Bube, 2004)*
  - Augmented MIB *(Feng, Long, Zhao, 2019)*

- **All existing methods are second order accurate**

Goal: Fourth order + Fast Poisson solver

- Fourth order augmented MIB (AMIB4)

• BVP without interface (*Feng, Zhao, JCP, 109391, 2020*).



• BVP with interface (*Feng, Zhao, JCP, 109677, 2020*).

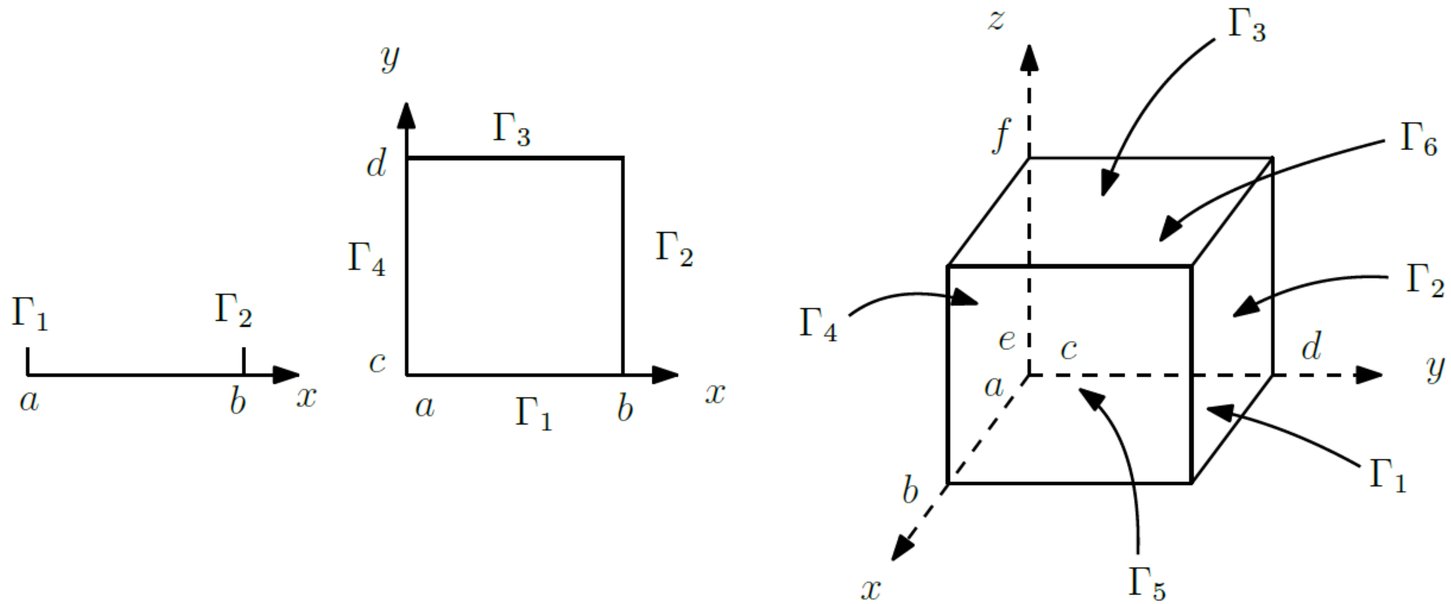
- Introduce auxiliary variables to preserve discrete Laplacian of central differences
- **FFT will not sense discontinuities**

2. Poisson boundary value problems

$$\Delta u = f(\vec{x}), \qquad (3)$$

subject to any boundary condition on Γ_j

1. Dirichlet: $u = \phi_j$
2. Neumann: $\dfrac{\partial u}{\partial n} = \phi_j$
3. Robin: $\dfrac{\partial u}{\partial n} + ku = \phi_j$



Fast Poisson Solvers

➢ **FISHPACK** *(Swarztrauber, Sweet)*

- The most widely used FFT-Poisson solver
- Second order central difference: $\{\frac{1}{h^2}, -\frac{2}{h^2}, \frac{1}{h^2}\}$
- Complexity in 3D: $O(n^3 \log n)$

$$u_{xx} = f, \qquad u(0) = u(1) = 0 \qquad (4)$$

1. Fast Sine transform (FST): $f \rightarrow \hat{f}$
2. $\hat{u} = \frac{\hat{f}}{\lambda}, \;\; \lambda_j = 4\, sin^2\left(\frac{j\pi}{n}\right)/(h^2)$
3. Inverse FST: $\hat{u} \rightarrow u$

FFT + fourth order central difference scheme

- Uniform grid: $\{x_0, x_1, \dots, x_n\}$
- Five points stencil: $\frac{1}{h^2}\{-\frac{1}{12}, \frac{4}{3}, -\frac{5}{2}, \frac{4}{3}, -\frac{1}{12}\}$

$$u_{xx} = f, \qquad u(0) = u(1) = 0 \qquad (4)$$

1. Fast Sine transform (FST): $f \to \hat{f}$
2. $\hat{u} = \frac{\hat{f}}{\lambda}, \;\; \lambda_j = -(\cos\left(\frac{j\pi}{n}\right) - 1)(\cos\left(\frac{j\pi}{n}\right) - 7)/(3h^2)$
3. Inverse FST: $\hat{u} \to u$

- Example 1

$u = \sin(4\pi x)$,
$f = 16\pi^2 \sin(4\pi x)$

- Example 2

$u = -\cos(4\pi x) + 1$,
$f = 16\pi^2 \cos(4\pi x)$

FFT vs LU decomposition

Example 1

N	FFT		LU	
	Error	Order	Error	Order
32	2.607E-4	–	2.607E-4	–
64	1.646E-5	3.99	1.646E-5	3.99
128	1.031E-6	4.00	1.031E-6	4.00
256	6.450E-8	4.00	6.450E-8	4.00
512	4.032E-9	4.00	4.032E-9	4.00

Example 2

N	FFT		LU	
	Error	Order	Error	Order
32	1.321E-2	–	5.229E-4	–
64	3.235E-3	2.03	3.294E-5	3.99
128	8.046E-4	2.00	2.063E-6	4.00
256	2.009E-4	2.00	1.290E-7	4.00
512	5.020E-5	2.00	8.061E-9	4.00

- **FFT degrades to second order in Example 2**

Anti-symmetric property

$$u(x_{-1}) = -u(x_1), \qquad u(x_{n+1}) = -u(x_{n-1}) \qquad (5)$$

- Example 1

$$u = \sin(4\pi x)\,,$$
$$f = 16\pi^2 \sin(4\pi x)$$

- Example 2

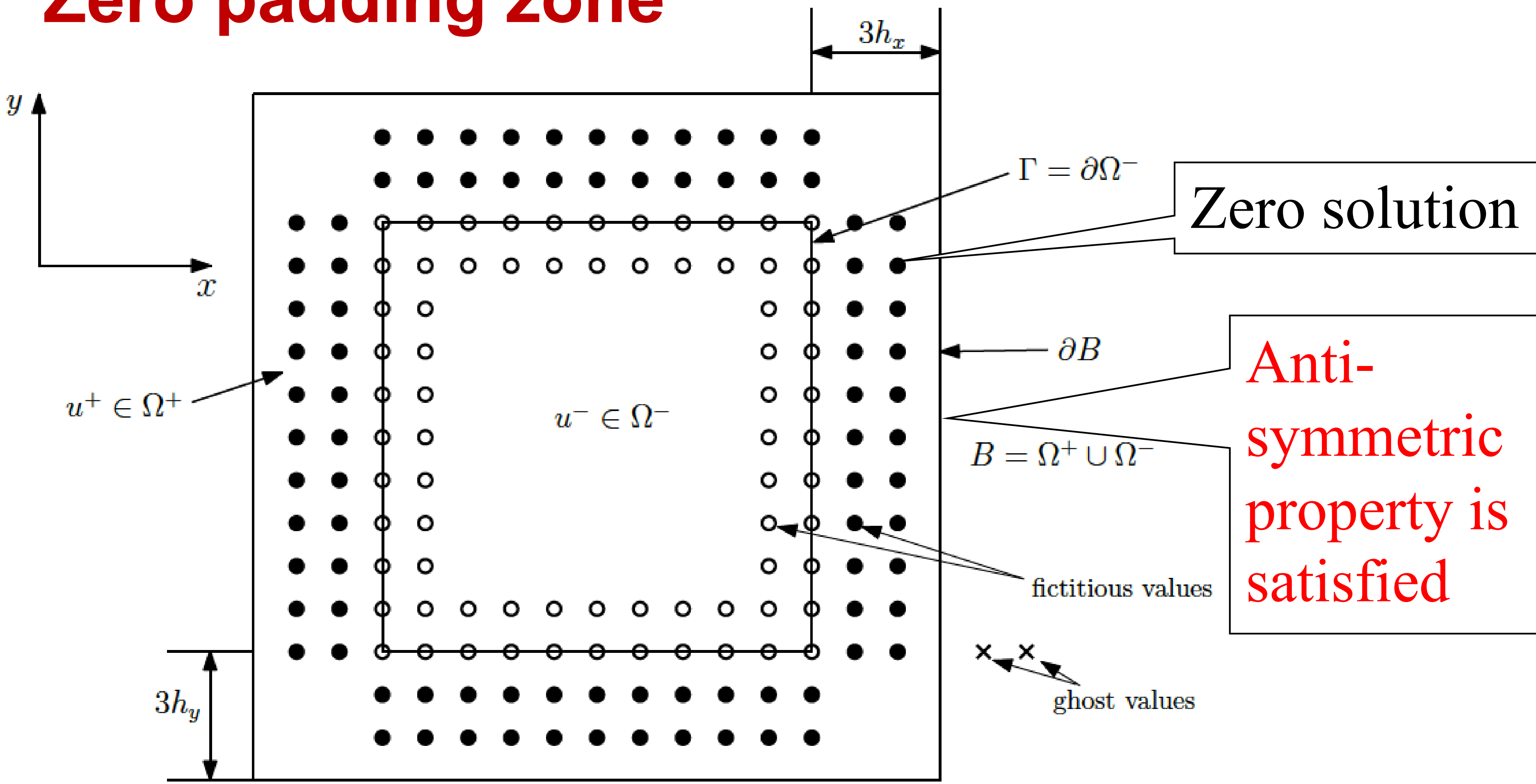
$$u = -\cos(4\pi x) + 1\,,$$
$$f = 16\pi^2 \cos(4\pi x)$$

- FFT degrades to second order, because (5) is not satisfied in Example 2

- **However, anti-symmetric property is invalid in general**

$$u_{xx} = f, \qquad u(0) = u(1) = 0 \qquad (4)$$

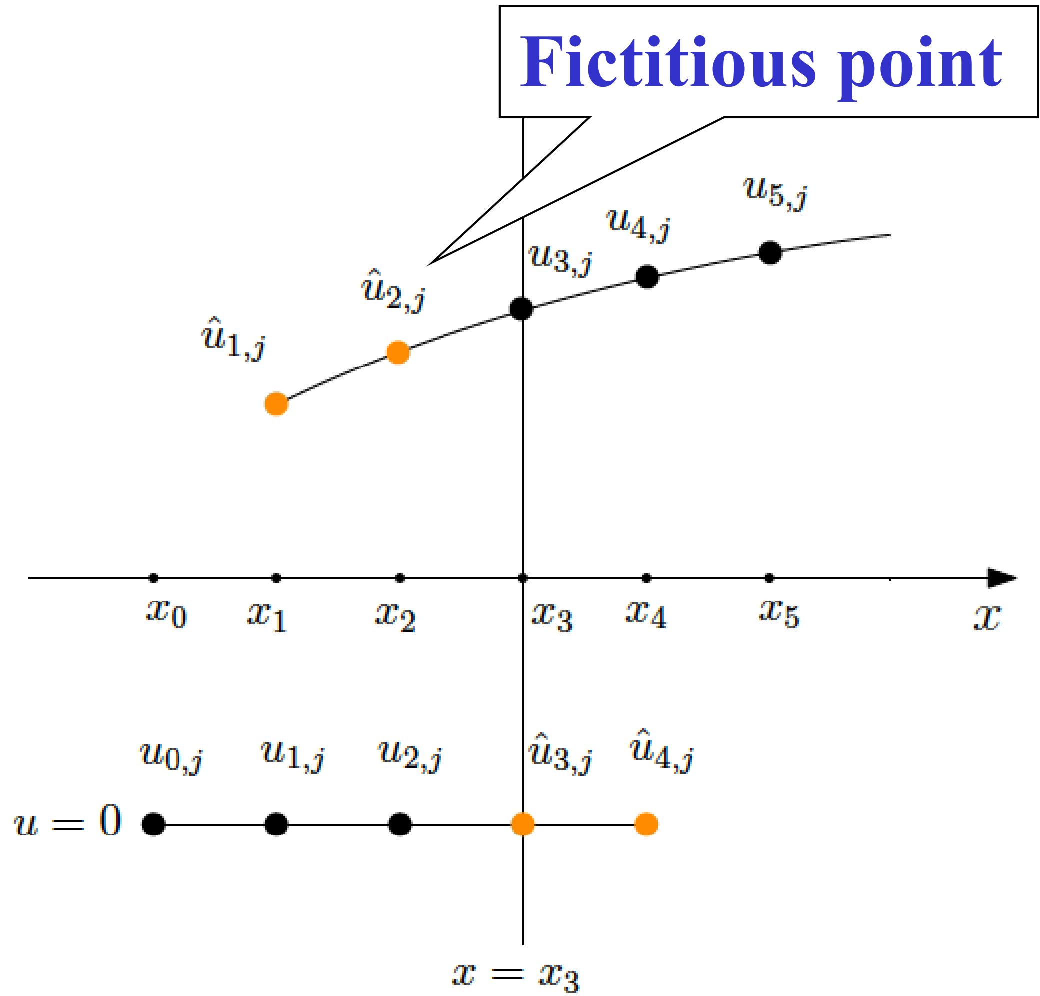
Zero padding zone



- Original boundary → immersed interface
- Boundary condition → interface condition

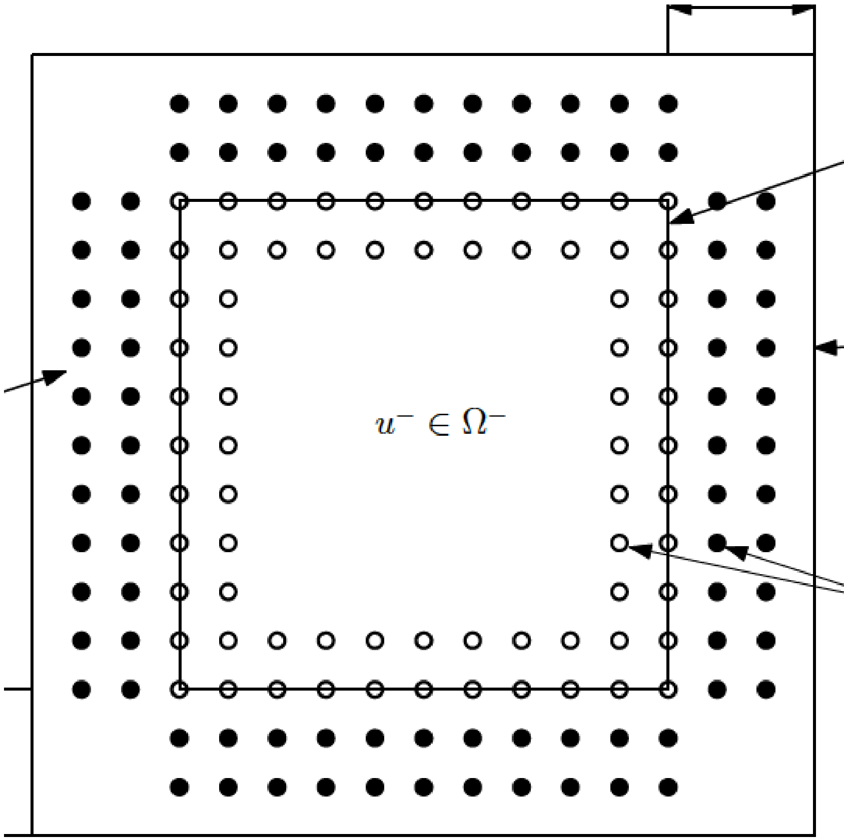
Matched interface and boundary (MIB) metho

- boundary condition: $$\frac{\partial u}{\partial x} + ku = \phi_3 \qquad (7)$$
- Second order MIB: Discretize (7) by using finite difference over $\{x_2, x_3, x_4\}$
- Solve fictitious value $\hat{u}_2$ as a linear combination of $\{u_3, u_4\}$ and ϕ_3
- High order: repeatedly enforce (7) to generate more fictitious values



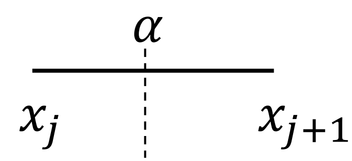
MIB fictitious value representation

- Two layers outside boundary for fourth order MIB
- A linear combination of some neighboring nodes and boundary values



$$\hat{u}_{i,j} = \sum_{(x_I, y_J) \in S_{i,j}} W_{I,J} u_{I,J} + W_0 \phi \,, \qquad (8)$$

Taylor expansion with jumps

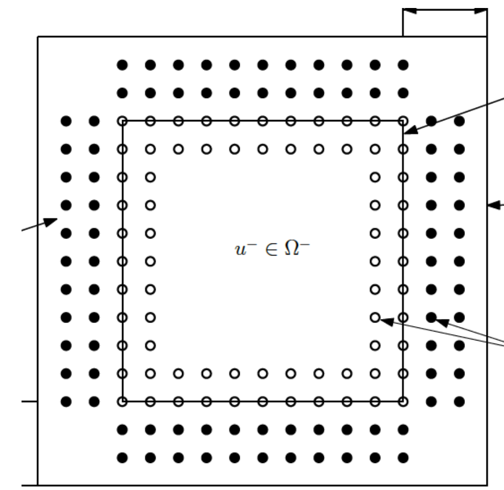


Theorem 1. Corrected fourth differences. Let $x_j \le \alpha < x_{j+1}, h^- = x_j - \alpha$, and $h^+ = x_{j+1} - \alpha$. Suppose $u \in C^6[x_j - 2h, \alpha) \bigcap C^6(\alpha, x_{j+1} + 2h]$, with derivative extending continuously up to the interface α. Then the following approximations hold to $O(h^4)$:

$$u_{xx}(x_{j-1}) \approx \frac{1}{h^2}[-\frac{1}{12}u(x_{j-3}) + \frac{4}{3}u(x_{j-2}) - \frac{5}{2}u(x_{j-1}) + \frac{4}{3}u(x_j) - \frac{1}{12}u(x_{j+1})] + \frac{1}{12h^2}\sum_{m=0}^{5}\frac{(h^+)^m}{m!}[u^{(m)}], \tag{22}$$

where $[u^{(m)}]$ are Cartesian derivative jumps

$$[\frac{\partial^m u}{\partial x^m}]|_{x=\alpha} = \lim_{x\to\alpha^+}\frac{\partial^m u}{\partial x^m} - \lim_{x\to\alpha^-}\frac{\partial^m u}{\partial x^m}$$



- Introduce Cartesian derivative jumps as auxiliary variables

$$Q := \{[u]_i, \left[\frac{\partial u}{\partial x}\right]_i, \left[\frac{\partial^2 u}{\partial x^2}\right]_i, \dots [u]_j, \left[\frac{\partial u}{\partial y}\right]_j, \left[\frac{\partial^2 u}{\partial y^2}\right]_j, \dots\}^T$$

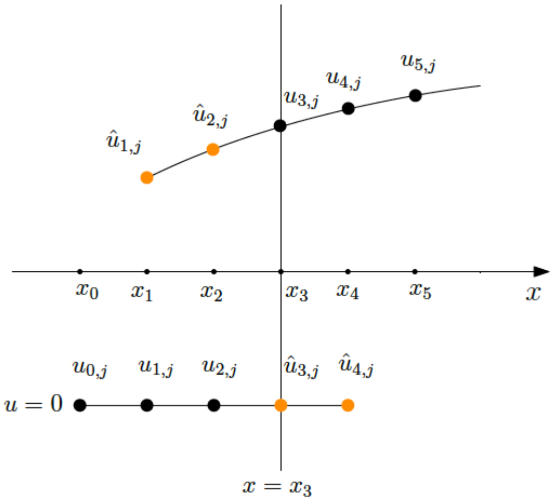
An augmented linear system

- Poisson equation (3) is discretized as

$$AU + BQ = F \qquad (9)$$

where *AU* is the discrete Laplacian generated by the 9-points fourth order central difference

- Reconstruct Cartesian derivative jumps by using fictitious values
- By eliminating fictitious values, Q linearly depends on U



$$CU + Q = \Phi \qquad (10)$$

A Schur complement procedure

$$\begin{aligned} AU + BQ &= F \\ CU + IQ &= \Phi \end{aligned} \qquad (11)$$

U: unknown solution; Q: auxiliary variable

- Solve a one-dimensionally smaller linear system iteratively

$$(\mathrm{I} - \mathrm{C}A^{-1}B)Q = \Phi - CA^{-1}F$$

- Then, solve U by one more FFT inversion

$$\mathrm{A}U = F - BQ$$

- FFT inversion complexity in 2D $\mathrm{O}(n^2 \log n)$

Fourth order MIB and AMIB

- 2D problem with Dirichlet boundaries
- AMIB=MIB+FFT, which is much faster than MIB

$[N_x, N_y]$	AMIB4					
	L_∞		L_2		CPU time(s)	iter no.
	Error	Order	Error	Order		
[11, 11]	4.408E-5	–	1.549E-5	–	4.823E-3	20
[27, 27]	1.096E-6	3.87	4.712E-7	3.65	1.290E-2	20
[59, 59]	4.662E-8	3.94	2.209E-8	3.81	4.056E-2	20
[123, 123]	2.442E-9	3.97	1.212E-9	3.90	0.139	21
[251, 251]	1.400E-10	3.98	7.111E-11	3.95	0.529	21
[507, 507]	7.771E-12	4.10	4.004E-12	4.08	2.403	21

$[N_x, N_y]$	MIB4				
	L_∞		L_2		CPU time(s)
	Error	Order	Error	Order	
[13, 13]	4.070E-5	–	1.841E-5	–	2.00E-3
[29, 29]	1.076E-6	4.28	5.267E-7	4.19	2.466E-2
[61, 61]	4.644E-8	4.12	2.345E-8	4.08	0.207
[125, 125]	2.444E-9	4.06	1.252E-9	4.04	1.836
[253, 253]	1.423E-10	4.00	7.329E-11	4.00	15.386
[509, 509]	3.363E-11	2.06	1.417E-11	2.34	148.41

Higher order AMIB

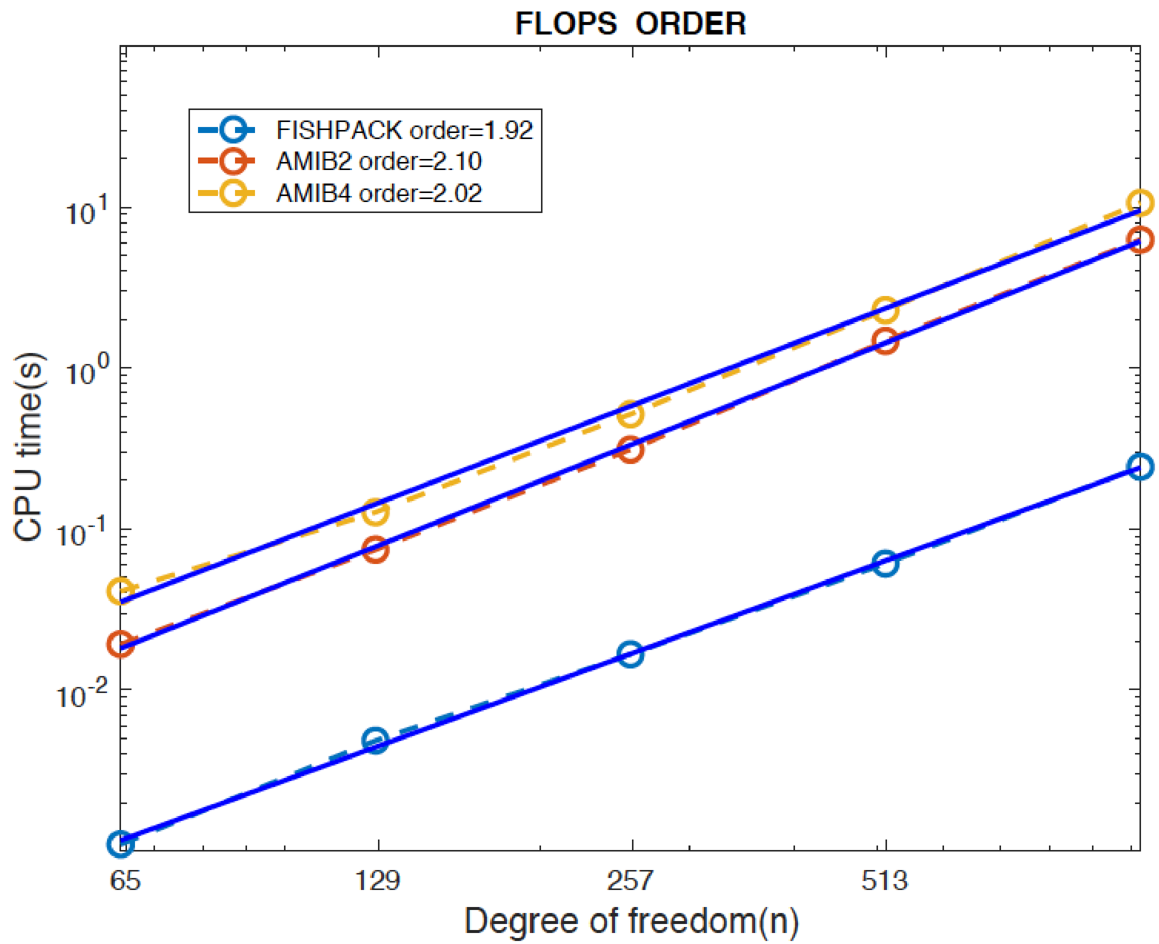
- Dirichlet, Robin, Robin, and Neumann

$[N_x, N_y]$	AMIB6 and $k = 10$				
	L_∞		L_2		
	Error	Order	Error	Order	
$[25, 25]$	1.072E-2	–	1.522E-3	–	32
$[57, 57]$	9.828E-5	5.54	1.640E-5	5.35	37
$[123, 123]$	9.412E-7	6.10	1.712E-7	5.98	40
$[249, 249]$	1.106E-8	6.12	2.119E-9	6.05	50
$[505, 505]$	1.489E-10	6.07	2.926E-11	6.04	69

$[N_x, N_y]$	AMIB8 and $k = 20$				
	L_∞		L_2		
	Error	Order	Error	Order	
$[23, 23]$	1.033	–	0.120	–	34
$[55, 55]$	2.589E-3	6.67	3.681E-4	6.44	42
$[121, 121]$	3.111E-6	8.60	2.575E-7	9.29	48
$[247, 247]$	1.724E-8	7.07	1.808E-9	6.74	56
$[503, 503]$	6.801E-11	7.76	8.209E-12	7.56	69

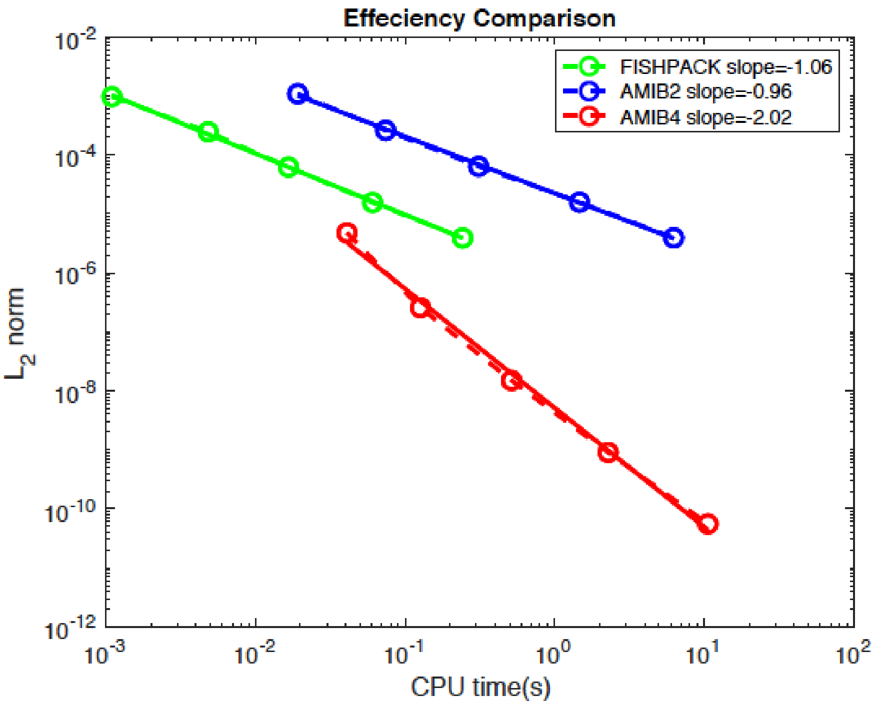
Efficiency in 2D

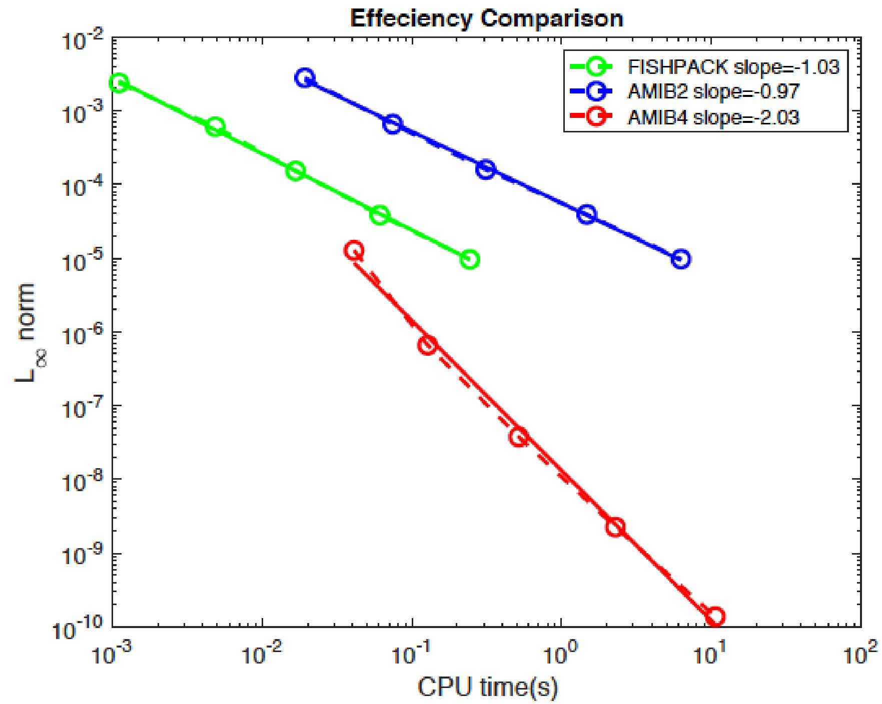
- FISHPACK *(Swarztrauber, Sweet)*
- AMIB: Performance is not optimized
- On the same mesh, AMIB2 and AMIB4 are more expensive than FISHPACK
- All: $O(n^2 \log n)$



Comparison with FISHPACK: cost-efficiency

- Plot error against CPU time





- **For a high precision, AMIB4 is more efficient that FISHPACK**
- Max error $= 10^{-10}$, FISHPACK is 10,000 times slower

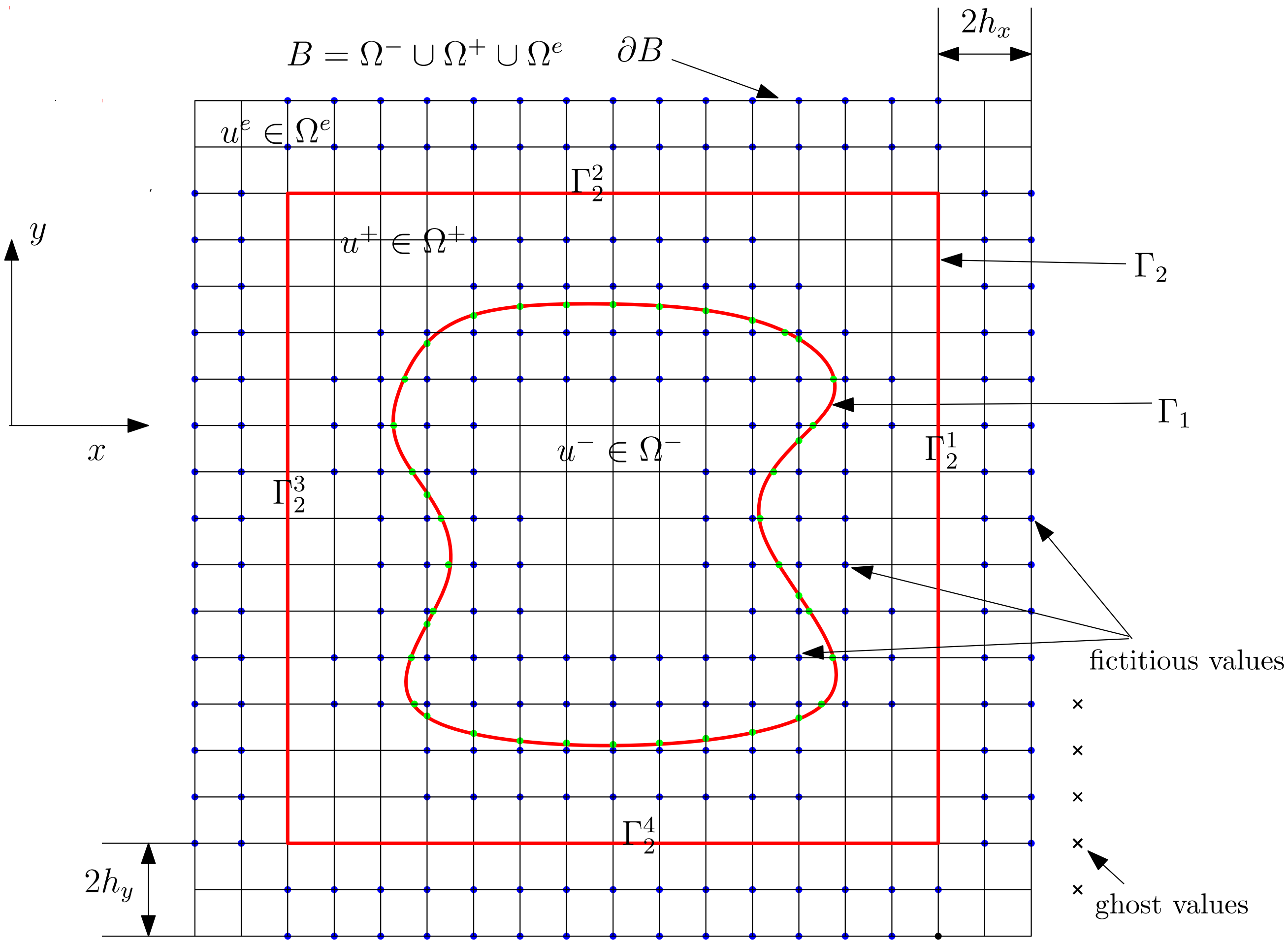
AMIB in 3D

- Dirichlet boundaries
- Tensor product type algorithm
- **Can be easily generalized to multi-dimensions**

$[N_x, N_y, N_z]$	AMIB4					
	L_∞		L_2		iter no.	CPU times(s)
	Error	Order	Error	Order		
[11, 11, 11]	0.870	–	0.127	–	37	4.722E-2
[27, 27, 27]	3.337E-2	3.81	3.347E-3	3.80	49	0.392
[59, 59, 59]	1.426E-3	4.13	1.216E-4	4.13	52	3.191
[123, 123, 123]	7.436E-5	4.10	5.760E-6	4.10	55	28.792
[251, 251, 251]	4.270E-6	4.06	3.132E-7	4.06	55	296.97

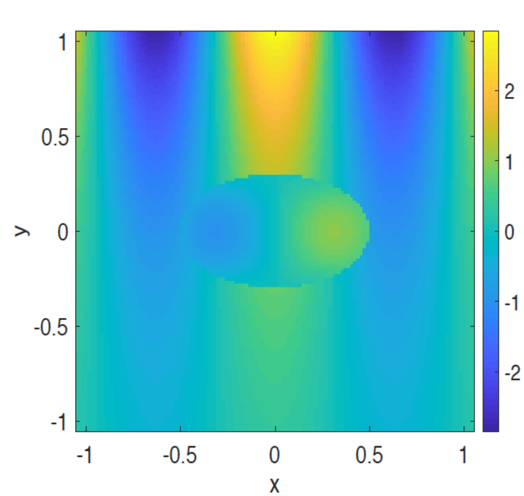
3. Elliptic interface problems in 2D

- Extend domain for FFT inversion
- MIB4 to handle interfaces and boundaries

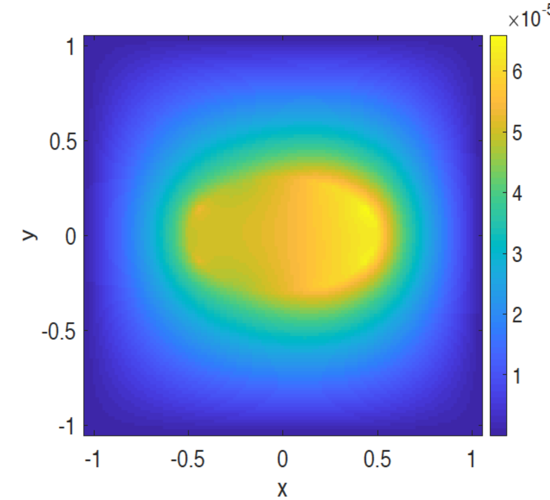


AMIB4 VS MIB4

- Fourth order
- AMIB is faster



Solution



Error

Table 5: Example 3b -$\beta^+ = 1, \beta^- = 10$; Ellipse interface; Robin boundary condition.

$[n, n]$	AMIB4					
	L_∞		L_2		iter no.	CPU time (s)
	Error	Order	Error	Order		
$[60, 60]$	1.647E-3	–	1.019E-3	–	39	3.967E-2
$[124, 124]$	1.132E-4	3.69	6.923E-5	3.70	62	0.171
$[252, 252]$	5.973E-6	4.15	3.559E-6	4.19	98	0.915
$[508, 508]$	4.264E-7	3.77	2.612E-7	3.73	141	5.387
$[n, n]$	MIB4					
	L_∞		L_2		iter no.	CPU time (s)
	Error	Order	Error	Order		
$[60, 60]$	1.190E-3	–	7.315E-4	–	509	0.115
$[124, 124]$	1.232E-4	3.12	7.559E-5	3.13	1286	0.803
$[252, 252]$	5.093E-6	4.49	3.000E-6	4.55	3366	8.47
$[508, 508]$	4.096E-7	3.60	2.506E-7	3.54	7569	79.53

Gradient recovery

- 4^{th} order in solution and gradient

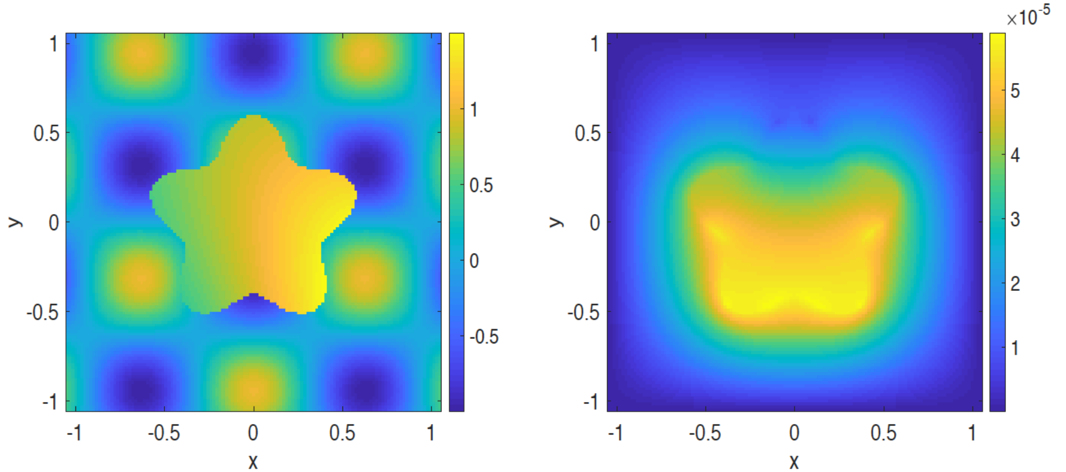
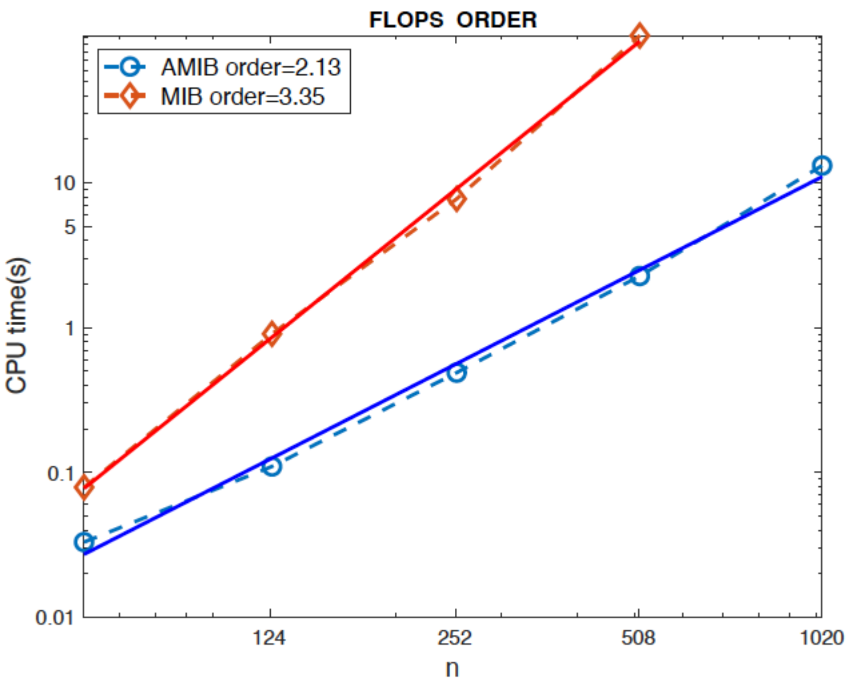


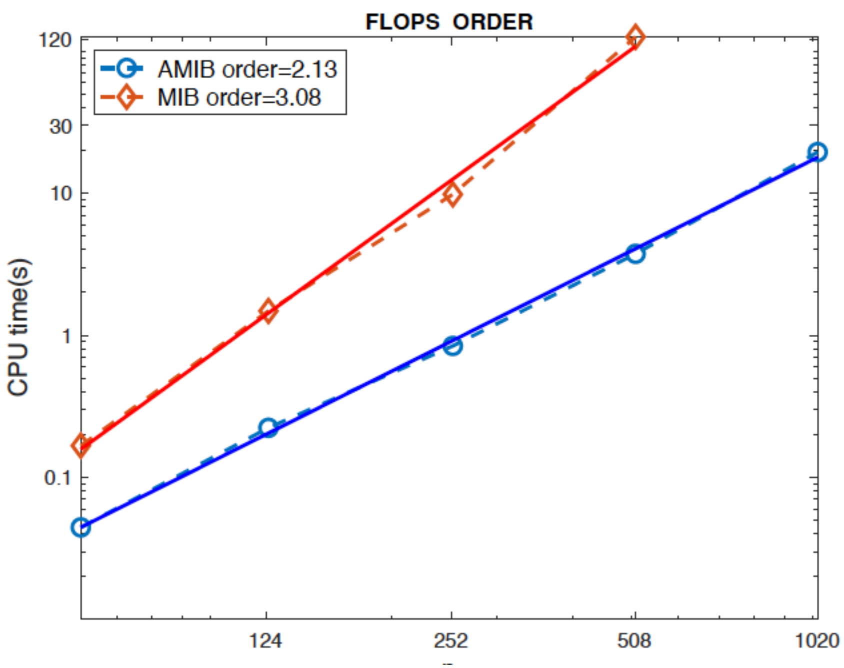
Table 7: Example 5 -$\beta^+ = 1, \beta^- = 20$; Five-leaf shaped interface.

$[n,n]$	AMIB4 L_∞ Error	L_∞ Order	L_2 Error	L_2 Order	iter no.	CPU time (s)
[60, 60]	1.078E-3	–	5.211E-4	–	43	4.442E-2
[124, 124]	5.885E-5	4.14	2.721E-5	4.13	70	0.223
[252, 252]	2.973E-6	4.06	1.229E-6	4.04	84	0.841
[508, 508]	9.272E-8	4.08	3.497E-8	4.08	100	3.744
[1020, 1020]	9.460E-9	2.76	2.263E-9	2.83	116	19.47
	Gradient L_∞ Error	L_∞ Order	L_2 Error	L_2 Order		
[60, 60]	4.824E-3	–	1.328E-3	–		
[124, 124]	2.300E-4	4.19	6.851E-5	4.08		
[252, 252]	3.221E-5	2.77	3.933E-6	4.03		
[508, 508]	8.286E-7	5.22	1.214E-7	4.96		
[1020, 1020]	3.586E-7	1.20	9.969E-9	3.59		

CPU time and efficiency for interface problem

- **MIB** $O(n^3)$
- **FFT-AMIB** $O(n^2)$ or $O(n^2 \log n)$





4. Summary

- Develop Augmented Matched Interface and Boundary (AMIB) method for solving elliptic PDEs
- **High order of accuracy**
  - 4^{th} – 8^{th} order accuracy for any boundary conditions
  - 4^{th} order accuracy for curve interfaces
- **High efficiency of the FFT**
  - $O(n^2 \log n)$ in 2D
  - $O(n^3 \log n)$ in 3D