

Algebraic Multigrid Techniques for the eXtended Finite Element Method

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Thanks to: E.Boman (Sandia), B.Hiriyur, H.Waisman (Columbia U.)

- Overview & Motivation
 - Why does standard SA-AMG fail & how to fix it
 - Examples
 - Conclusion



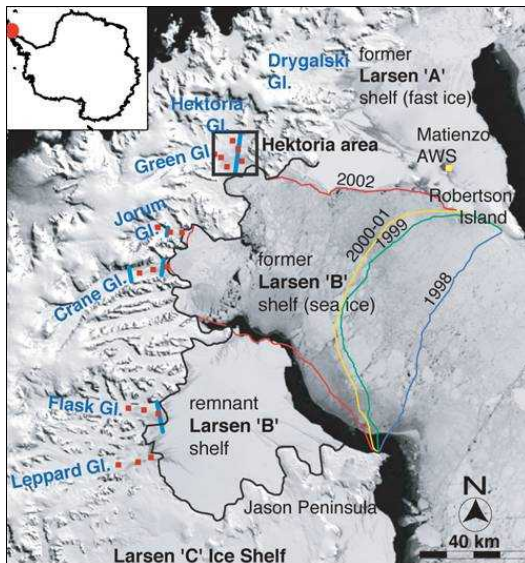
eXtended Finite Element Method (XFEM)

- allows to treat problems with singularities or discontinuities that are 'impractical' to be resolved by h-adaptivity. (*adapted from Wikipedia*)
- does so by extending the approximation space with known analytic solutions – similar to p-adaptivity, but not the same.
- has been applied to 3d
 - Crack propagation
 - Fluid-structure interaction
 - Multi-material problems and multi-phase flow
 - ...
- could be termed: 'fixed-grid method', 'embedded discontinuity method', 'partition of unity method', ...

Fracture of ice

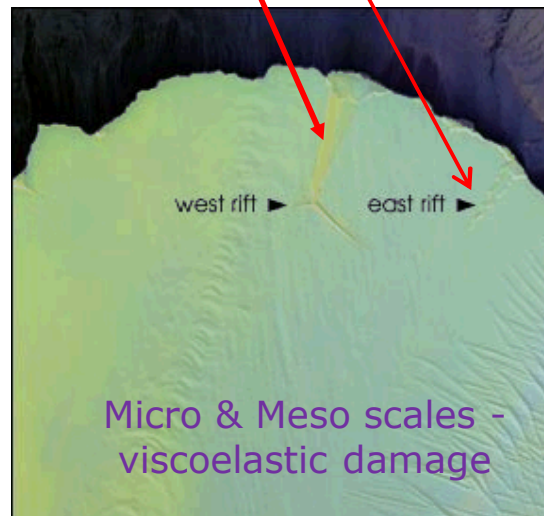
- Objective:** Employ parallel computers to better understand how fracture of land ice affects the global climate. Fracture happens e.g. during
- the collapse of ice shelves,
 - the calving of large icebergs, and
 - the role of fracture in the delivery of water to the bed of ice sheets.

Ice shelves in Antarctica:

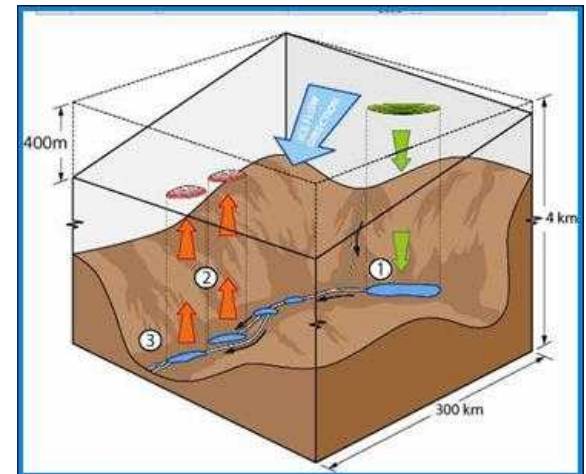


Larsen 'B' diminishing shelf
1998-2002
Other example: Wilkins ice shelf 2008

Macro scale - rifts will be represented by cracks (XFEM)



Amery ice shelf

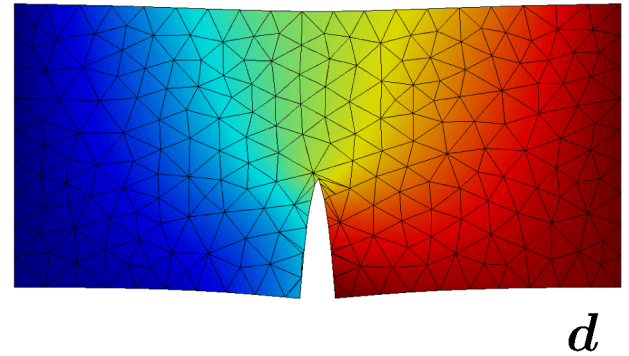


Glacial hydrology
(Source: <http://www.sale.scar.org>)

Computational Modeling of Fracture

Classical FEM approach to fracture mechanics

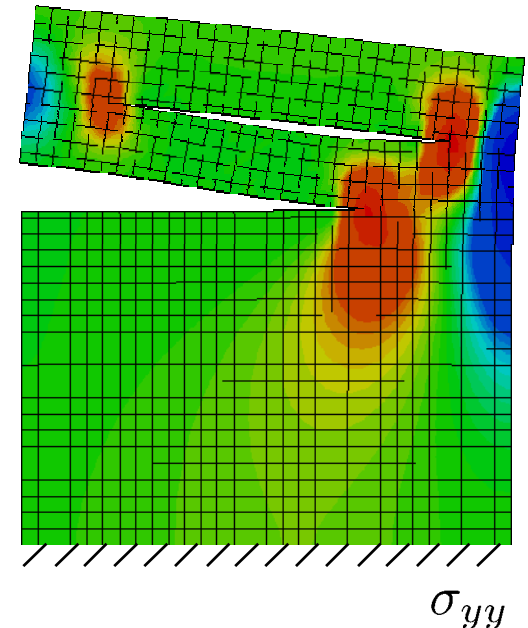
- Mesh conforms to crack boundaries
- Crack propagation → remeshing at each step
 - Requires fine mesh for tip singularities
 - Mesh smoothing for 'ugly' elements



eXtended Finite Element Method (XFEM)*

- Base mesh independent of crack geometry
- Crack propagation → adding “enriched” DOF with special basis functions to existing nodes
 - Number of DOFs change, mesh does not
 - Crack geometry defined through levelsets
 - Enrichments have local support

* Belytschko & Black (1999), Moes et al. (1999)



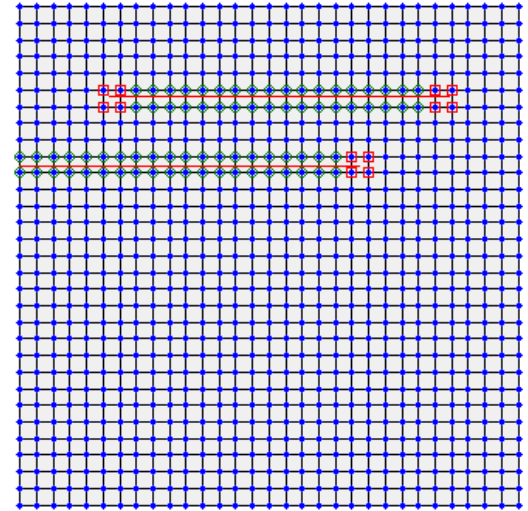
XFEM Formulation for Cracks

Displacement approximation (shifted basis form.)

$$u^h(\mathbf{x}) = \sum_{I=1}^n N_I(\mathbf{x}) u_I$$

$$\blacksquare + \sum_{i=1}^{n_h} N_{I_i}(\mathbf{x}) (H(\mathbf{x}) - H(\mathbf{x}_{I_i})) a_{I_i}$$

$$\blacksquare + \sum_{i=1}^{n_f} N_{\hat{I}_i}(\mathbf{x}) \sum_{J=1}^{n_J} (F_J(\mathbf{x}) - F_J(\mathbf{x}_{\hat{I}_i})) b_{\hat{I}_i J}$$



- Jump Enrichment
- Tip Enrichment (brittle crack)

$$H(\mathbf{x}) = \begin{cases} 0.5 & \text{in } \Omega^+ \\ -0.5 & \text{in } \Omega^- \end{cases}$$

$$F_J(r, \theta) = \left\{ \overbrace{\sqrt{r} \sin\left(\frac{\theta}{2}\right)}^{J=1}, \overbrace{\sqrt{r} \cos\left(\frac{\theta}{2}\right)}^{J=2}, \overbrace{\sqrt{r} \sin\left(\frac{\theta}{2}\right) \sin(\theta)}^{J=3}, \overbrace{\sqrt{r} \cos\left(\frac{\theta}{2}\right) \sin(\theta)}^{J=4} \right\}$$

→ Bubnov-Galerkin method: use identical approximation for test function $\delta \mathbf{d}(\mathbf{x})$

Global system

$$\mathbf{A} = \sum_e \int_{\Omega_e} \mathbf{B}_e^T \mathbf{C} \mathbf{B}_e d\mathbf{x}$$

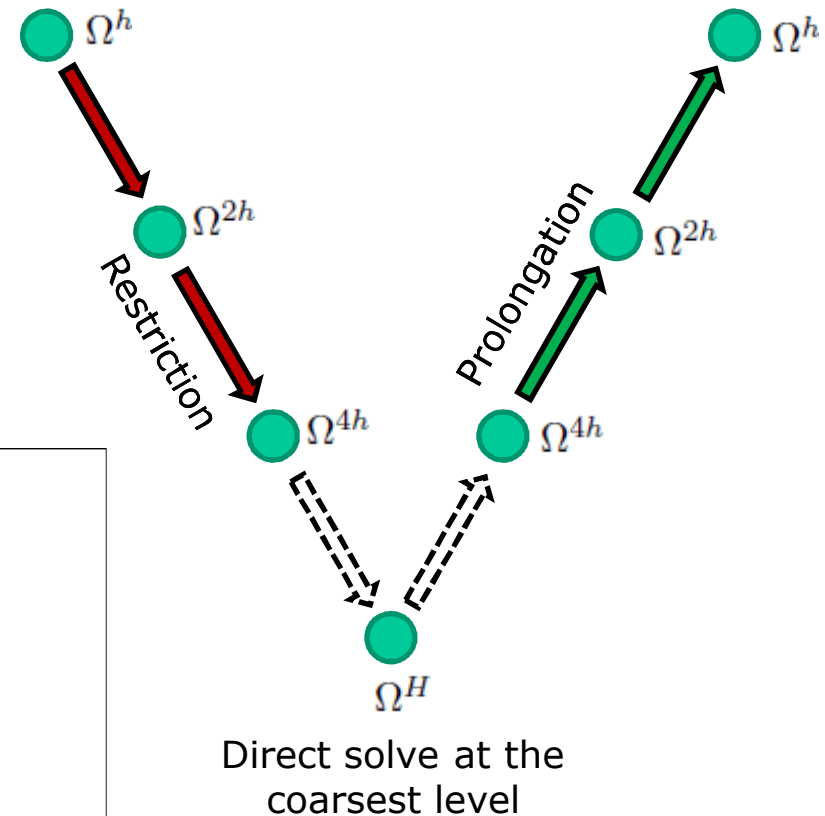
$$\mathbf{f} = \sum_e \int_{\Gamma_e} \mathbf{N}_e^T h d\mathbf{x} + \sum_e \int_{\Omega_e} \mathbf{N}_e^T \rho d\mathbf{x}$$

$$\mathbf{A} \mathbf{u} = \mathbf{f}$$

Multigrid principles

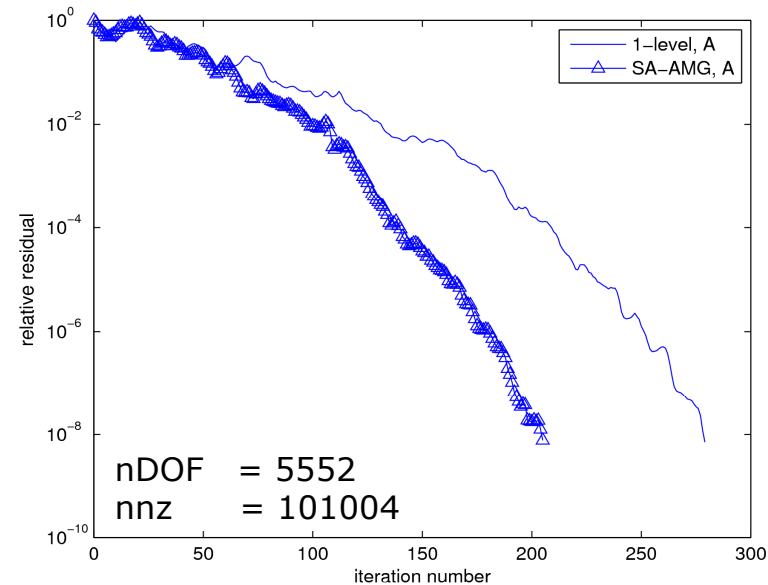
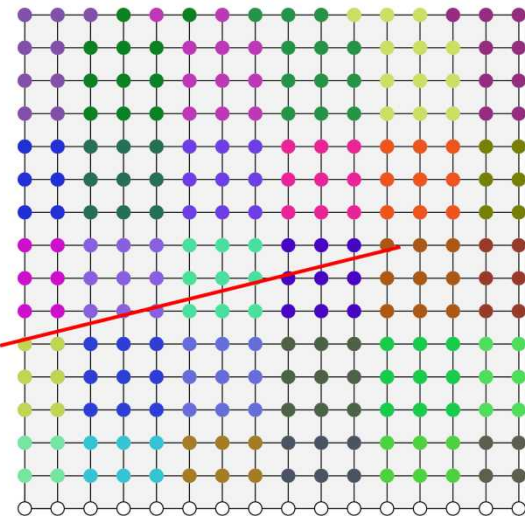
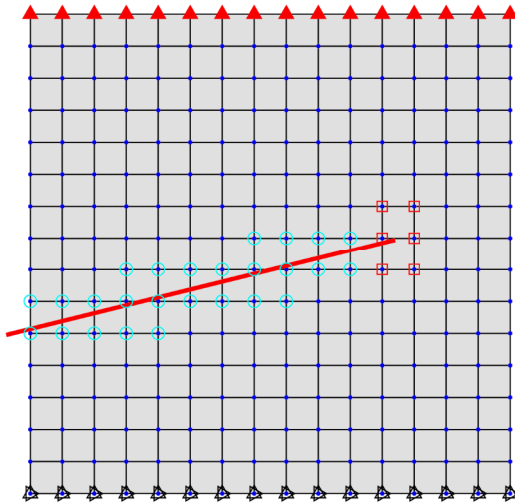
- Oscillatory components of error are reduced effectively by smoothing, but smooth components attenuate slower
- Key idea \rightarrow capture error at multiple resolutions using grid transfer operators $R^{[k]}$ and $P^{[k]}$
- **In AMG**, transfer operators are obtained from **graph information of A**
- Interpolation complements relaxation

```
// Solve  $A^{[k]}u^{[k]} = b^{[k]}$ 
procedure multilevel( $b^{[k]}, u^{[k]}, k$ )
   $u^{[k]} = \mathcal{R}^{[k]}(A^{[k]}, b^{[k]}, u^{[k]});$ 
  if ( $k \neq \ell$ )
     $r^{[k]} = b^{[k]} - A^{[k]}u^{[k]} ;$ 
     $u^{[k+1]} = 0;$ 
     $u^{[k+1]} = \text{multilevel}((P^{[k]})^T r^{[k]}, u^{[k+1]}, k+1);$ 
     $u^{[k]} = u^{[k]} + P^{[k]}u^{[k+1]};$ 
     $u^{[k]} = \mathcal{R}^{[k]}(A^{[k]}, b^{[k]}, u^{[k]});$ 
```

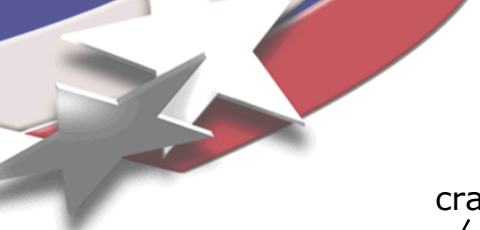


Recursive multigrid V Cycle consisting of l cycles to solve $Au=b$

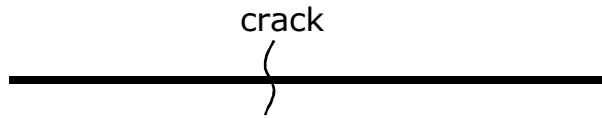
'Standard' SA-AMG for fracture problems



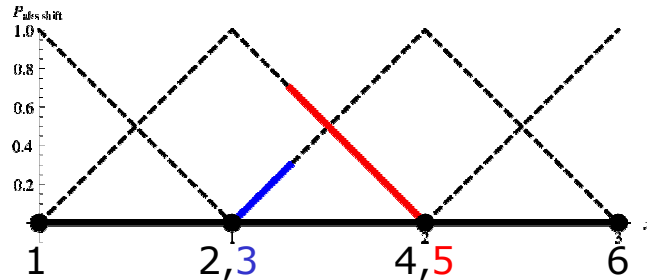
- Aggregation
 - Aggregates should not cross crack
- Nullspace
 - Elasticity: 3 ZEMs
 - Uncoupled domains: 6 ZEMs or more?
- Assumption of 2 unknowns per node fails
 - 2, 4, or 10 DOFs per node



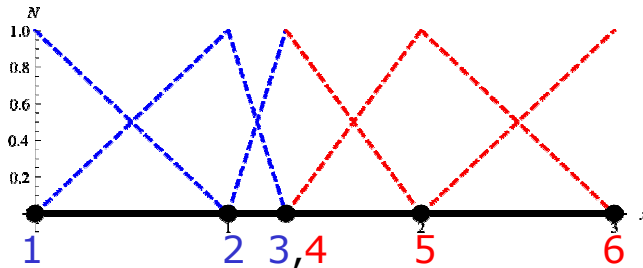
Distinct region representation



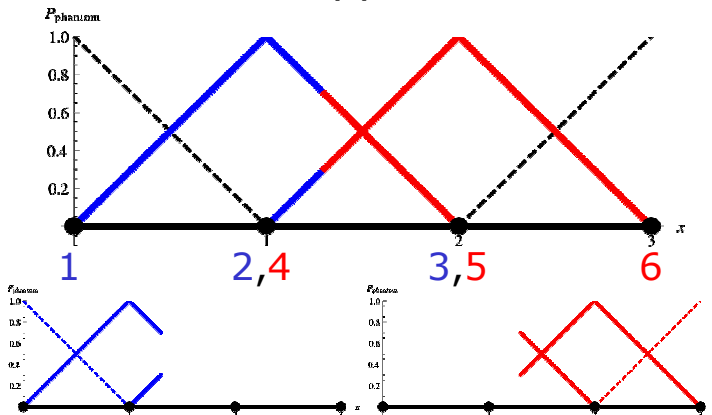
XFEM: modified shifted enrichment



FEM



Phantom node approach



$$\mathbf{K} \quad \mathbf{M}$$

$$u^h(x) = \sum_I N_I(x) |H(x) - H(x_I)| u_I$$

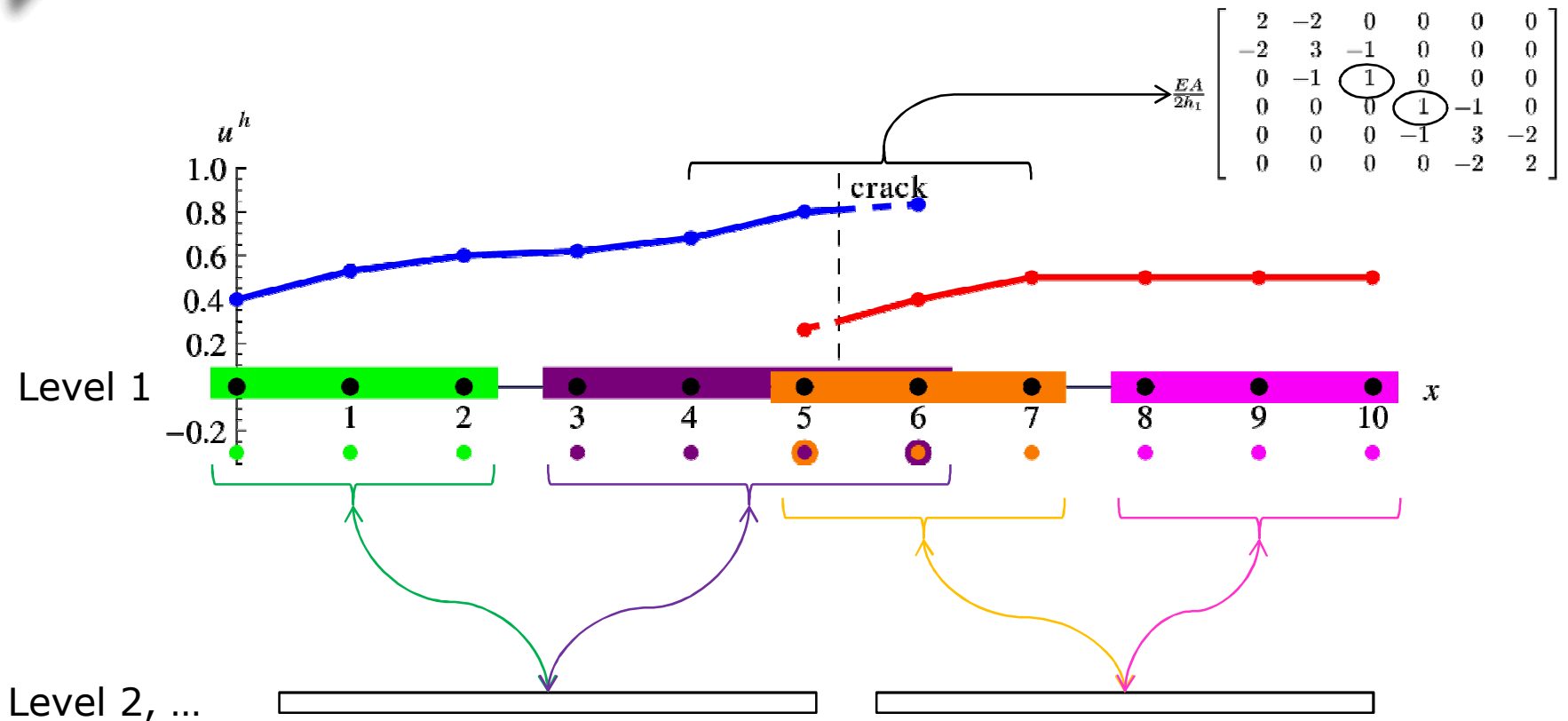
$$\frac{EA}{2h_1} \begin{bmatrix} 2 & -2 & 0 & 0 & 0 & 0 \\ -2 & 4 & 1 & -2 & -1 & 0 \\ 0 & 1 & 1 & -1 & 0 & 0 \\ 0 & -2 & -1 & 4 & 1 & -2 \\ 0 & -1 & 0 & 1 & 1 & 0 \\ 0 & 0 & 0 & -2 & 0 & 2 \end{bmatrix} \quad \frac{\rho A h_1}{24} \begin{bmatrix} 8 & 4 & 0 & 0 & 0 & 0 \\ 4 & 16 & 1 & 4 & 2 & 0 \\ 0 & 1 & 1 & 2 & 0 & 0 \\ 0 & 4 & 2 & 16 & 1 & 4 \\ 0 & 2 & 0 & 1 & 1 & 0 \\ 0 & 0 & 0 & 4 & 0 & 8 \end{bmatrix}$$

$$\frac{EA}{2h_1} \begin{bmatrix} 2 & -2 & 0 & 0 & 0 & 0 \\ -2 & 6 & -4 & 0 & 0 & 0 \\ 0 & -4 & 4 & 0 & 0 & 0 \\ 0 & 0 & 0 & 4 & -4 & 0 \\ 0 & 0 & 0 & -4 & 6 & -2 \\ 0 & 0 & 0 & 0 & -2 & 2 \end{bmatrix} \quad \frac{\rho A h_1}{24} \begin{bmatrix} 8 & 4 & 0 & 0 & 0 & 0 \\ 4 & 12 & 2 & 0 & 0 & 0 \\ 0 & 2 & 4 & 0 & 0 & 0 \\ 0 & 0 & 0 & 4 & 2 & 0 \\ 0 & 0 & 0 & 2 & 12 & 4 \\ 0 & 0 & 0 & 0 & 4 & 8 \end{bmatrix}$$

$$\frac{EA}{2h_1} \begin{bmatrix} 2 & -2 & 0 & 0 & 0 & 0 \\ -2 & 3 & -1 & 0 & 0 & 0 \\ 0 & -1 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & -1 & 0 \\ 0 & 0 & 0 & -1 & 3 & -2 \\ 0 & 0 & 0 & 0 & -2 & 2 \end{bmatrix} \quad \frac{\rho A h_1}{24} \begin{bmatrix} 8 & 4 & 0 & 0 & 0 & 0 \\ 4 & 15 & 2 & 0 & 0 & 0 \\ 0 & 2 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 2 & 0 \\ 0 & 0 & 0 & 2 & 15 & 4 \\ 0 & 0 & 0 & 0 & 4 & 8 \end{bmatrix}$$

(reordered for visualization)

Aggregation for phantom nodes: 1D

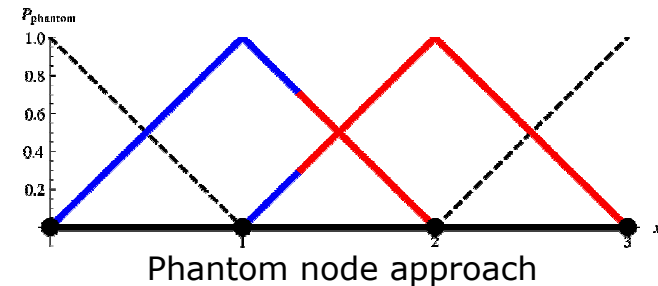
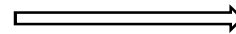
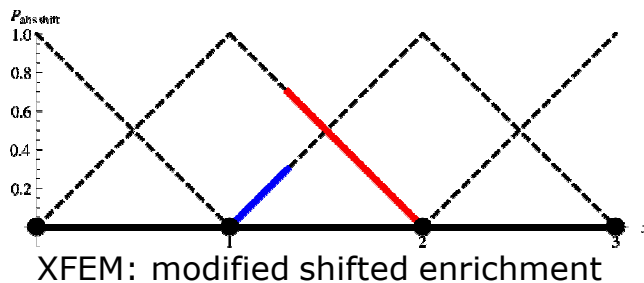


Aggregates seemingly overlap, but are **not** connected on any level!

Do XFEM developers have to use the phantom node approach? No!

For each node I with jump DOFs:

$$\phi_I - \bar{\phi}_I = \phi_\alpha$$

$$\bar{\phi}_I = \bar{\phi}_\alpha$$


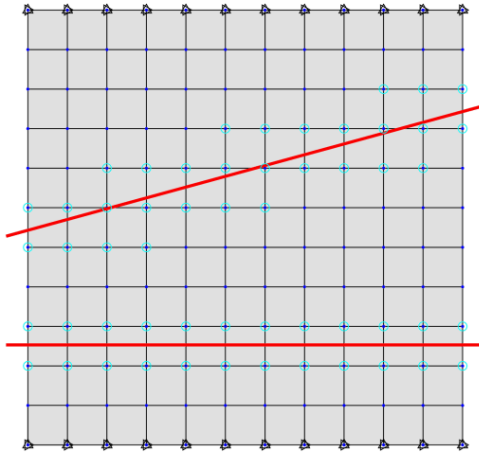
$$G^T \cdot A \cdot G \cdot G^{-1} \cdot u = G^T \cdot f$$

G

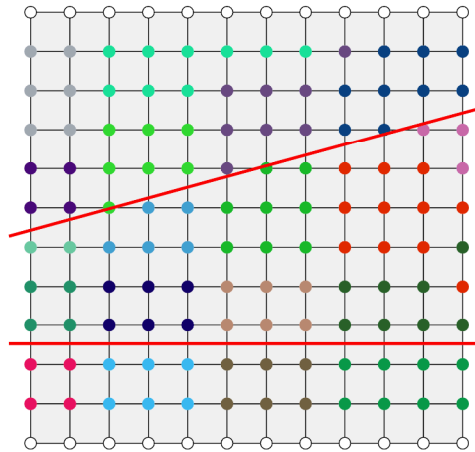
- is extremely sparse,
- is simple to produce,
- transformations are processor-local,
- applies only to jump DOFs
- exists for higher order Lagrange Polynomials and multiple dimensions

$$G^T = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & -1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & -1 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix}$$

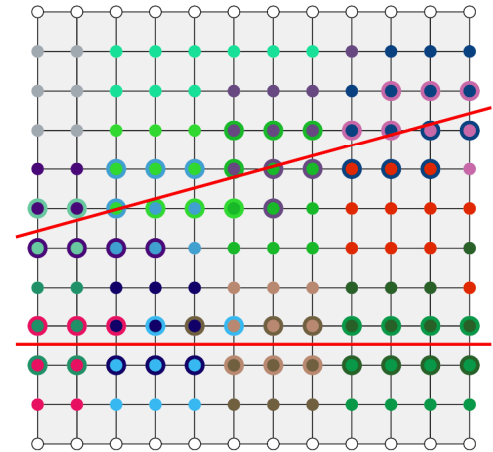
Aggregation for phantom nodes: 2D



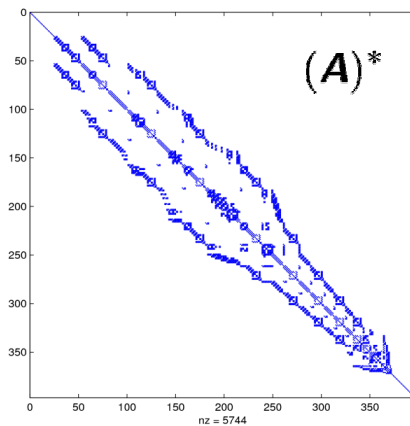
Mesh + Enrichment



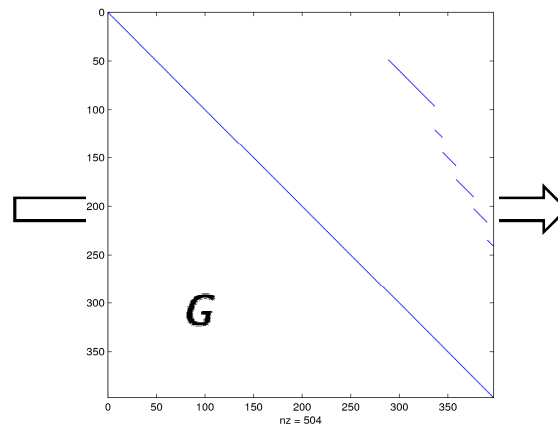
Standard DOFs only



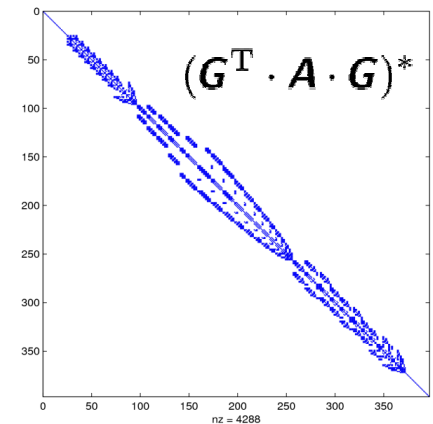
Standard + Jump DOFs



Modified shifted enrichment



$$G^T \cdot A \cdot G \cdot G^{-1} \cdot u = G^T \cdot f$$



Phantom node approach

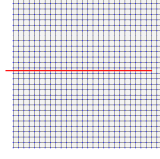
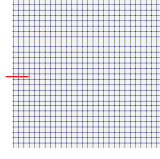
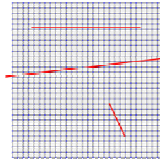
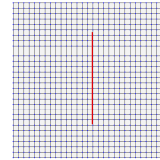
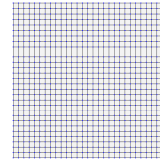
()* \rightarrow sym. rev. Cuthill-McKee permutation

Prelim. results for jump enrichments only

A Shifted enrichment

$G^T \cdot A \cdot G$ Phantom node

If one wants to use the standard graph-based aggregation, then using Phantom node setup is crucial!



Case	$n_e \times n_e$	$\alpha_{\text{cond.}}$	n_{iter}			
			A		$G^T \cdot A \cdot G$	
			1L	ML	1L	ML
I	30×30	3e+03	32	9	32	9
	60×60	1e+04	63	10	63	10
	90×90	3e+04	93	11	93	11
	120×120	5e+04	123	11	123	11
II	30×30	2e+06	59	40	53	12
	60×60	1e+06	109	58	104	13
	90×90	2e+06	159	65	156	14
	120×120	1e+07	-	81	-	15
III	30×30	1e+04	46	25	42	11
	60×60	5e+04	86	33	83	13
	90×90	1e+05	127	40	127	15
	120×120	2e+05	170	44	167	15
1a	30×30	1e+05	54	16	54	11
	60×60	4e+05	106	21	105	14
	90×90	1e+06	157	24	157	16
	120×120	2e+06	-	26	-	16
1c	30×30	2e+07	78	38	76	16
	60×60	7e+07	150	53	146	17
	90×90	1e+08	-	63	-	18
	120×120	2e+08	-	73	-	21

SA-OC: 1.28-1.40

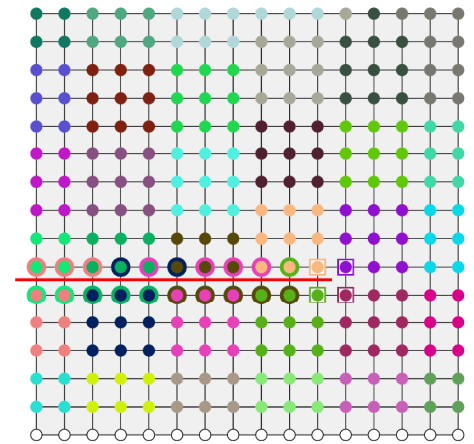
NullSpace for Jump & Tip Enrichments

2D Elasticity problem has 3 zero energy modes

	1	2	3
Dx_I	1	...	-y_I
Dy_I	0	1	x_I
		...	

Nullspace for phantom node setup

- Standard DOFs are treated as usual
- Phantom DOFs are treated like Standard DOFs
 - Put '1' into x- and y- displacement col.
 - Put coordinate into the rotation column
- Consider extra tip DOFs as fine-scale features
 - They don't contribute to the rigid body motion
 - put 0 into their respective rows
 - → no coarse level contribution in prolongation & restriction
 - → smoothing only on finest level



$$+ \sum_{i=1}^{n_f} N_{\hat{f}_i}(\mathbf{x}) \sum_{J=1}^{n_J} \left(F_J(\mathbf{x}) - F_J(\mathbf{x}_{\hat{f}_i}) \right) b_{\hat{f}_i J} \quad F_J(r, \theta) = \left\{ \overbrace{\sqrt{r} \sin\left(\frac{\theta}{2}\right)}^{J=1}, \overbrace{\sqrt{r} \cos\left(\frac{\theta}{2}\right)}^{J=2}, \overbrace{\sqrt{r} \sin\left(\frac{\theta}{2}\right) \sin(\theta)}^{J=3}, \overbrace{\sqrt{r} \cos\left(\frac{\theta}{2}\right) \sin(\theta)}^{J=4} \right\}$$

- Don't transform tip dofs!

- Finest Level: Combine standard (Block-) Gauss-Seidel smoothing with special tip smoother D^{tip}

- Tip smoother: let \mathcal{T} contain all extra enriched tip DOFs. Then

$$D_{\mathcal{T}\mathcal{T}}^{\text{tip}} = \tilde{A}_{\mathcal{T}\mathcal{T}}^{-1}$$

$$D_{ij}^{\text{tip}} = 0 \text{ if } i \notin \mathcal{T} \text{ or } j \notin \mathcal{T}$$

- Pre-smoother:

$$u \leftarrow \text{GaussSeidel}(u, \tilde{A}, b)$$

$$u \leftarrow u + D^{\text{tip}} \cdot (b - \tilde{A} \cdot u)$$

- Post-smoother

$$u \leftarrow u + D^{\text{tip}} \cdot (b - \tilde{A} \cdot u)$$

$$u \leftarrow \text{GaussSeidel}(u, \tilde{A}, b)$$

Pre-Post-smoother symmetry is important

Reason for special smoothing:

- dense blocks (40x40 for quad4)
- high condition number

- All coarser levels: standard GaussSeidel
- Coarsest Level: Direct solve

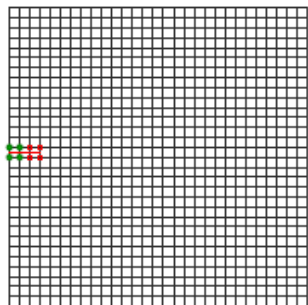
Numerical Results...

Test Cases:

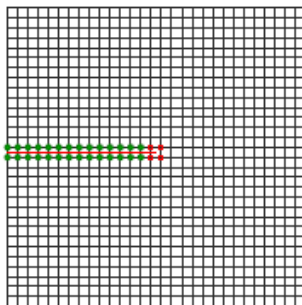
- Both edge cracks and interior cracks considered
- CG preconditioned with AMG
 - VBlk AMG: block form of standard AMG with 1 pre + 1 post **block** sym(GS)
 - Hybrid Standard AMG: $P(A_{rr}, A_{rr})$ with 1 pre + 1 post sym(GS) on 2x2 system
 - Quasi-AMG: $P(A_{rr}, \hat{A}_{rr})$ with 1 pre + 1 post sym(GS) on 2x2 system

Single Propagating Crack

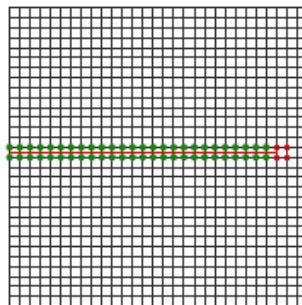
Two Cracks



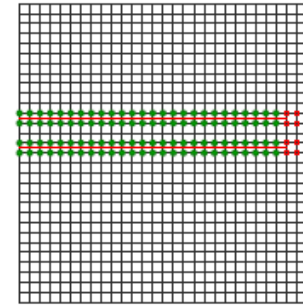
(a) Case 1a



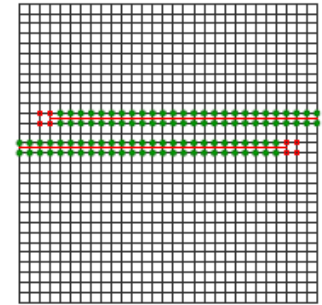
(b) Case 1b



(c) Case 1c



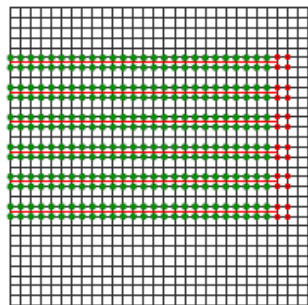
(d) Case 2a



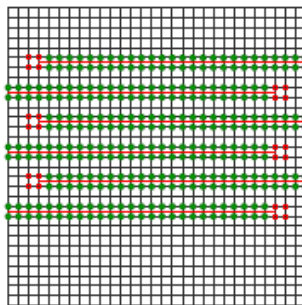
(e) Case 2b

Six Cracks

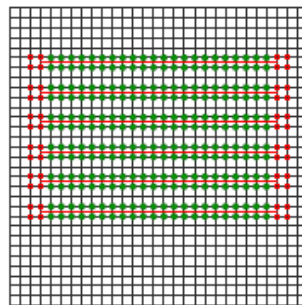
Inclined Cracks



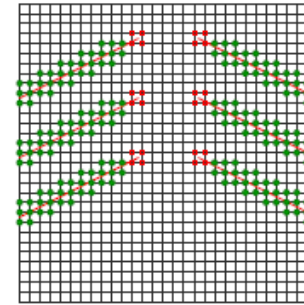
(f) Case 3a



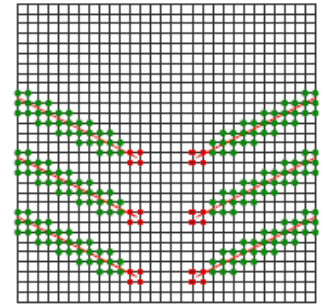
(g) Case 3b



(h) Case 4



(i) Case 5a



(j) Case 5b

Numerical Results for full XFEM system



Without cracks



Case	$n_e \times n_e$	n_{iter}									$\alpha_{cond.}$
		1L	ML		ML, MS		ML, NS		ML, MS, NS		
			SA	EM	SA	EM	SA	EM	SA	EM	
I	30×30	33	8	8	8	8	8	8	8	8	3e+03
	60×60	64	10	11	10	11	10	11	10	11	1e+04
	90×90	94	11	12	11	12	11	12	11	12	3e+04
II	30×30	160	138	130	25	29	111	112	19	21	3e+07
	60×60	-	-	-	31	38	191	180	24	26	2e+09
	90×90	-	-	-	31	42	-	-	21	31	9e+09
	120×120	-	-	-	144	-	-	-	28	40	7e+10
III	30×30	116	88	78	21	19	79	70	18	14	3e+07
	60×60	-	120	99	24	23	102	86	20	17	8e+08
	90×90	-	148	138	27	27	115	102	22	20	1e+10
	120×120	-	162	153	29	27	120	107	24	21	4e+10
1a	30×30	66	31	30	16	15	31	29	16	15	6e+05
	60×60	117	31	30	18	17	31	30	18	16	3e+06
	90×90	165	33	29	20	16	33	30	20	16	1e+07
	120×120	-	32	31	19	17	32	31	19	16	2e+07
1c	30×30	86	34	37	21	24	34	37	20	23	1e+08
	60×60	157	35	41	23	28	35	40	23	28	7e+08
	90×90	-	35	41	24	29	35	42	24	29	2e+09
	120×120	-	37	44	26	31	37	44	26	31	3e+09

# of levels	full complexity	(1,1) complexity
2	1.673	1.607
3	1.815	1.716
3	1.65	1.583
4	1.699	1.621

SA-OC: 1.28-1.40

EM-OC: 1.13-1.17

Numerical Results for full XFEM system



Without cracks



Case	$n_e \times n_e$	n_{iter}									$\alpha_{cond.}$
		1L	ML		ML, MS		ML, NS		ML, MS, NS		
			SA	EM	SA	EM	SA	EM	SA	EM	
I	30×30	33	8	8	8	8	8	8	8	8	3e+03
	60×60	64	10	11	10	11	10	11	10	11	1e+04
	90×90	94	11	12	11	12	11	12	11	12	3e+04
II	30×30	160	138	130	25	29	111	112	19	21	3e+07
	60×60	-	-	-	31	38	191	180	24	26	2e+09
	90×90	-	-	-	31	42	-	-	21	31	9e+09
	120×120	-	-	-	144	-	-	-	28	40	7e+10
III	30×30	116	88	78	21	19	79	70	18	14	3e+07
	60×60	-	120	99	24	23	102	86	20	17	8e+08
	90×90	-	148	138	27	27	115	102	22	20	1e+10
	120×120	-	162	153	29	27	120	107	24	21	4e+10
1a	30×30	66	31	30	16	15	31	29	16	15	6e+05
	60×60	117	31	30	18	17	31	30	18	16	3e+06
	90×90	165	33	29	20	16	33	30	20	16	1e+07
	120×120	-	32	31	19	17	32	31	19	16	2e+07
1c	30×30	86	34	37	21	24	34	37	20	23	1e+08
	60×60	157	35	41	23	28	35	40	23	28	7e+08
	90×90	-	35	41	24	29	35	42	24	29	2e+09
	120×120	-	37	44	26	31	37	44	26	31	3e+09

# of levels	full complexity	(1,1) complexity
2	1.673	1.607
3	1.815	1.716
3	1.65	1.583
4	1.699	1.621

Remove emin,
remove OC (make it a comment below)

SA-OC: 1.28-1.40

EM-OC: 1.13-1.17

Todo:

Show conditioning?

Pictures of test cases?

Add a convergence diagram to support table



Concluding Remarks

Standard SA-AMG methods can be used, if proper input is provided!

- Key components:
 - System matrix must be in phantom-node form
 - Either you already have it, (voids, fluid-structure interaction, ...) , or
 - do a simple transformation $\mathbf{G}^T \cdot \mathbf{A} \cdot \mathbf{G} \cdot \mathbf{G}^{-1} \cdot \mathbf{u} = \mathbf{G}^T \cdot \mathbf{f}$
 - Adapt nullspace with zero entries for extra tip DOFs
 - Two-step smoothing on finest level

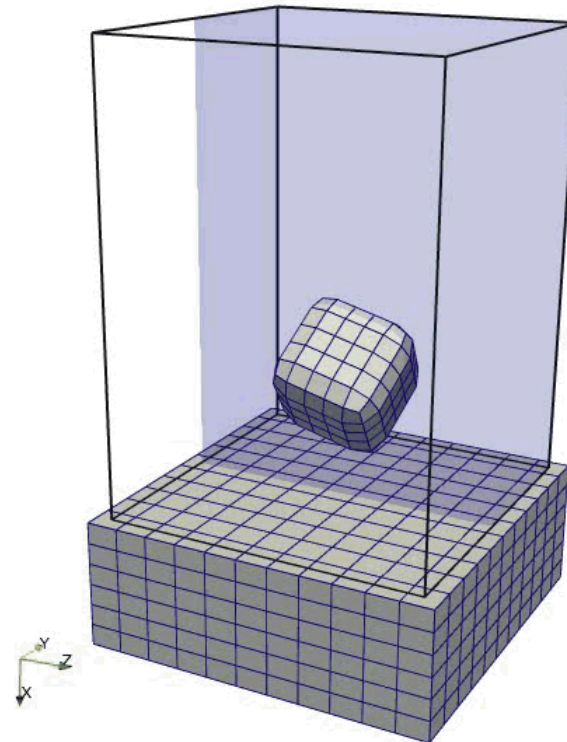
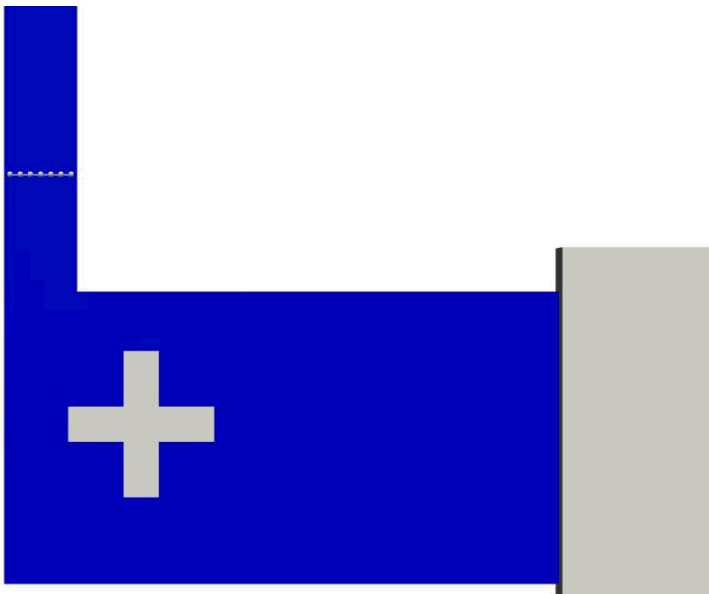
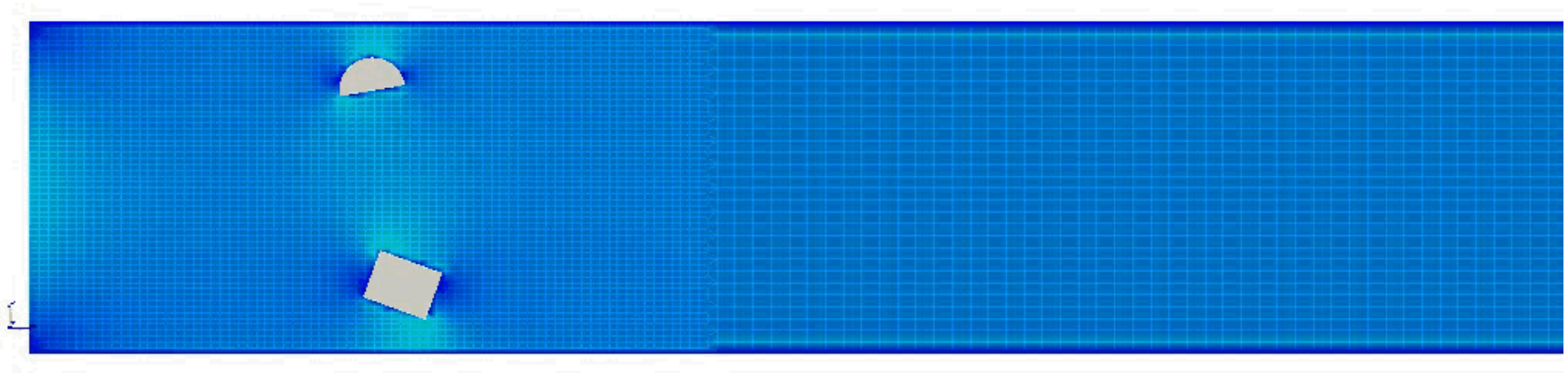
Future Directions

- 3d implementation
- What happens to tiny element fractions (conditioning)?
- Can we get even closer to pure FEM?

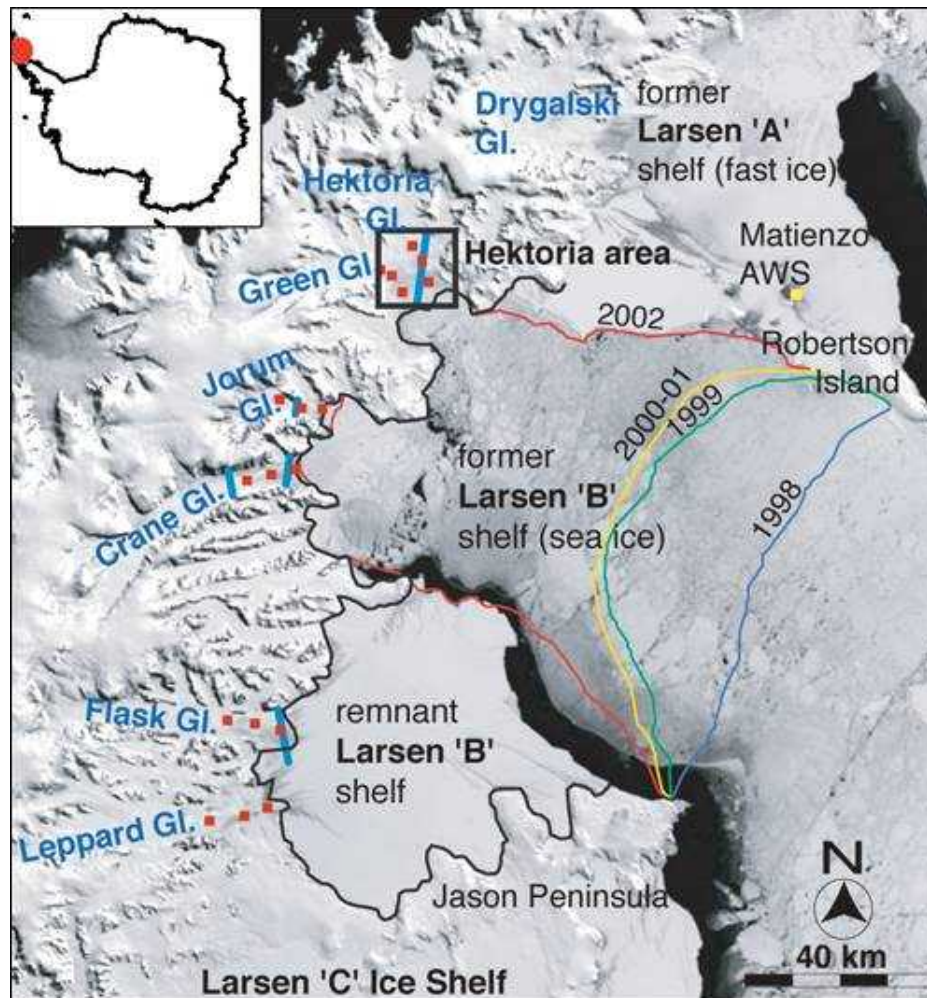
Backup slides

XFEM flow and fluid-structure interaction

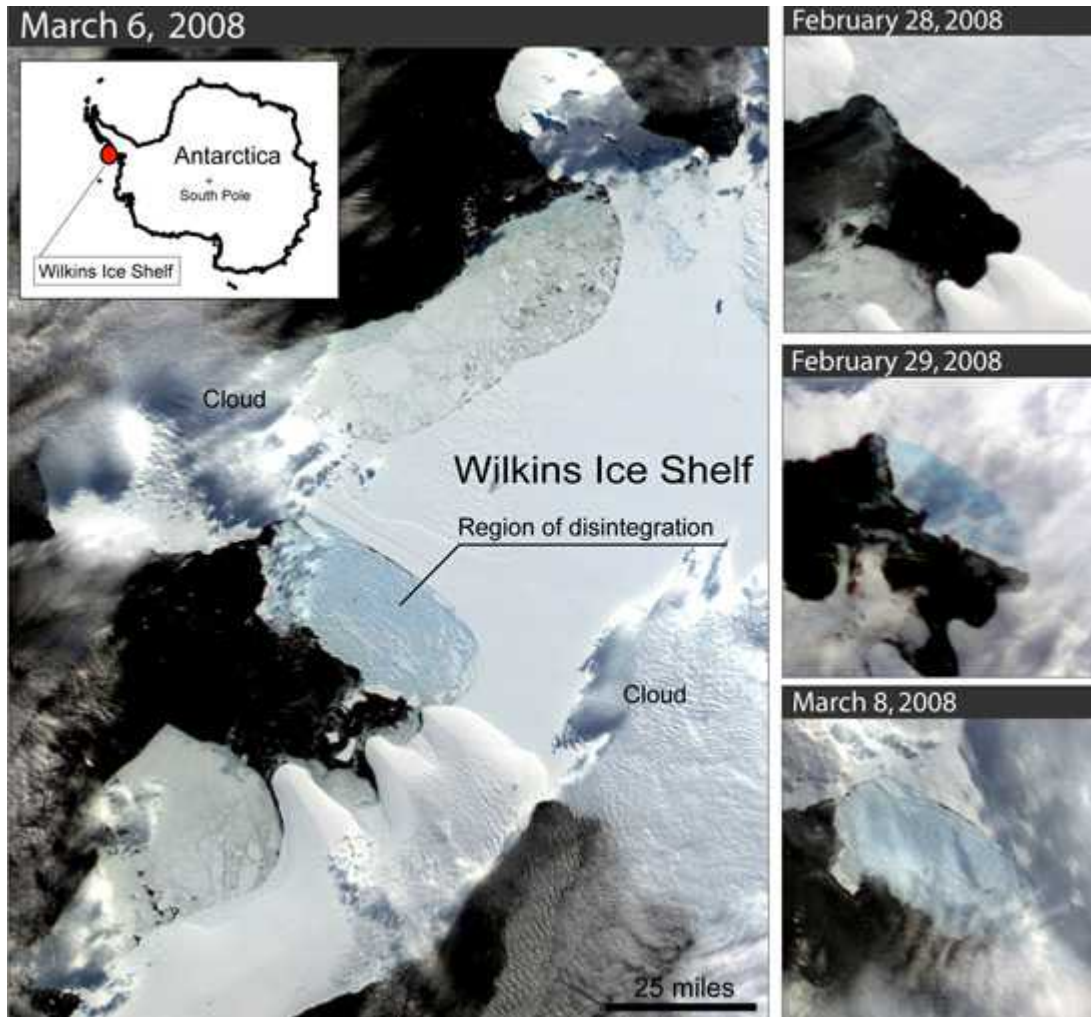
A. Gerstenberger, "An XFEM based fixed-grid approach to fluid-structure interaction", PhD thesis, 2010



Larsen 'B' shelf, 1998-2002



Wilkins ice shelf, 2008



Computational Modeling of Fracture

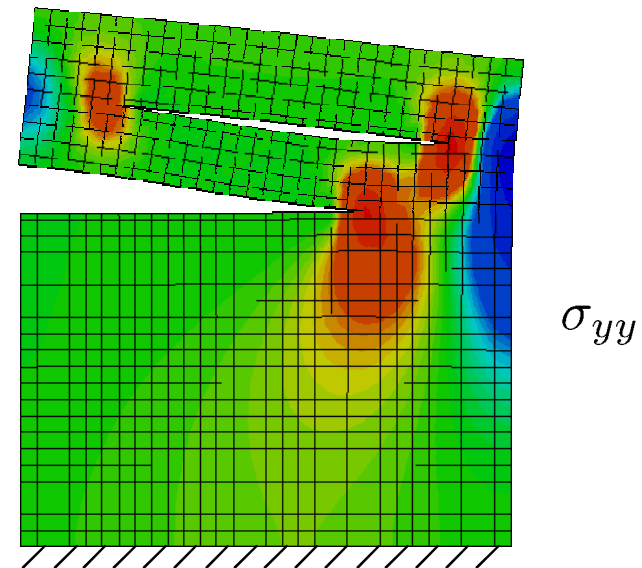
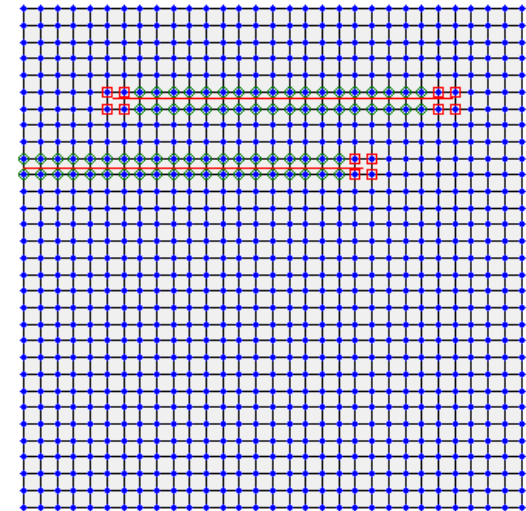
Classical FEM approach to fracture mechanics

- Mesh conforms to crack boundaries
- Crack propagation → remeshing at each step
 - Requires double-nodes for crack opening and fine mesh for tip singularities

eXtended Finite Element Method (XFEM)*

- Base mesh independent of crack geometry
- Crack propagation → adding “enriched” DOF with special basis functions to existing nodes
 - Crack geometry defined through levelsets
 - Discontinuities and singularities captured through special basis functions (enrichments)
 - Enrichments have local support

XFEM mesh



* Belytschko & Black (1999), Moes et al. (1999)

XFEM Linear system

Strain-displacement relation:

$$\mathbf{B}_{enr}^e = \nabla_{sym} \mathbf{N}_{enr}^e$$

- Symmetric gradient operator applied to enriched basis-function matrix



Weak form

Stiffness matrix:

$$\mathbf{A}_e = \int_{\Omega_e} (\mathbf{B}_{enr}^e)^T \mathbf{D} \mathbf{B}_{enr}^e d\Omega_e$$

- Numerical quadrature for stiffness matrix



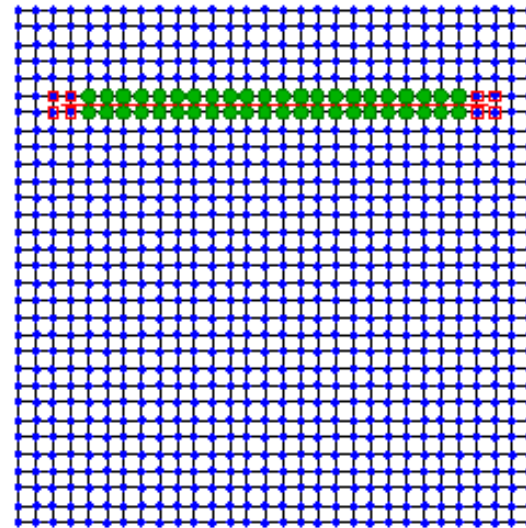
Assembly

XFEM Linear System:

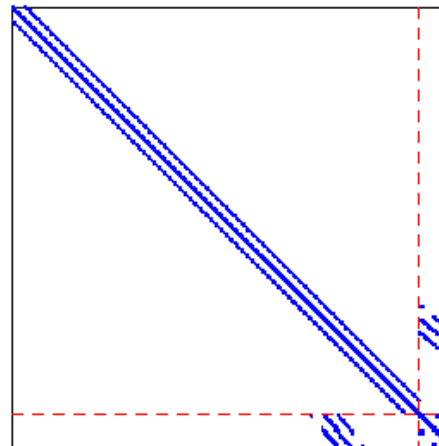
$$\begin{bmatrix} A_{rr} & A_{rx} \\ A_{xr} & A_{xx} \end{bmatrix} \begin{bmatrix} u_r \\ u_x \end{bmatrix} = \begin{bmatrix} \tilde{f}_r \\ \tilde{f}_x \end{bmatrix}$$

- Enriched DOF grouped together at the end in u_x
- A_{xx} small compared to A_{rr} for relatively small number of cracks

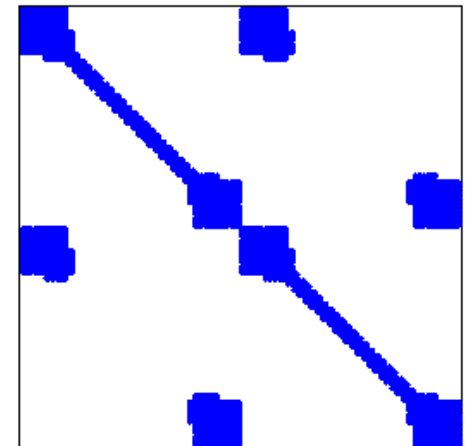
XFEM mesh



Sparsity pattern of A



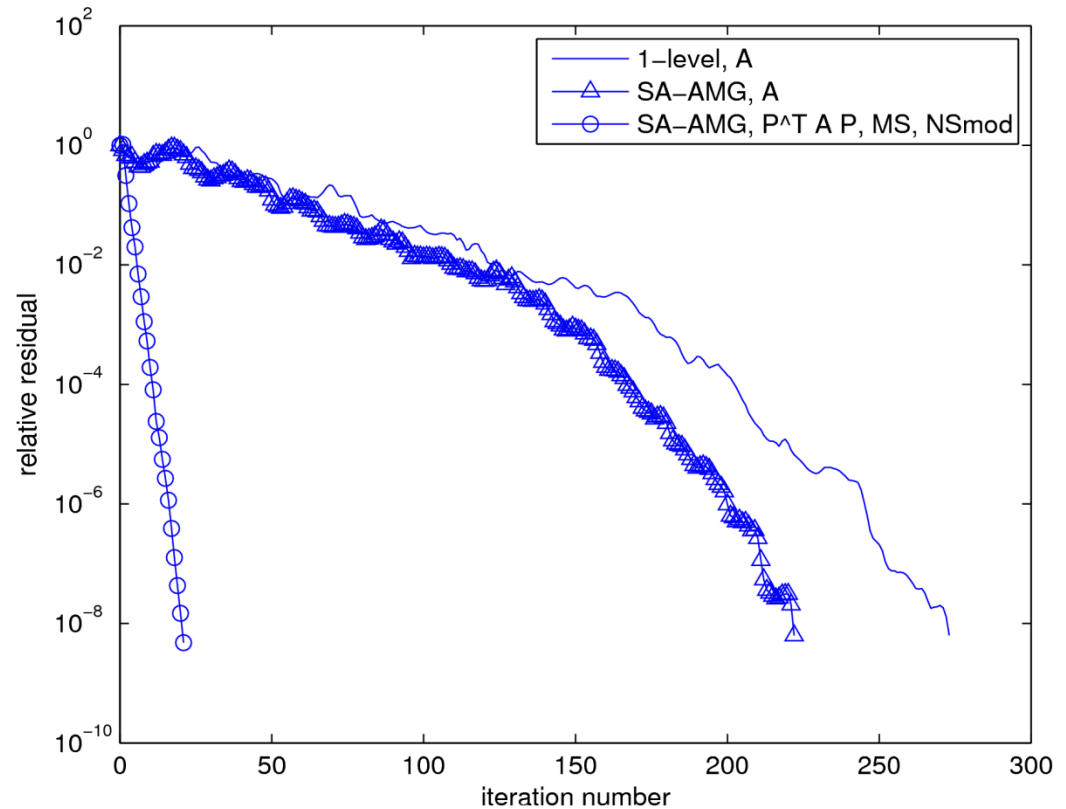
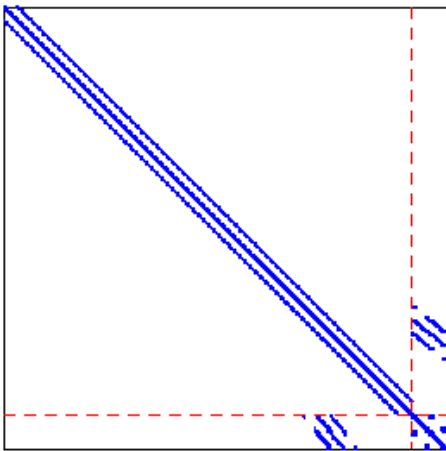
Sparsity pattern of A_{xx}



'Standard' SA-AMG for elastic problems

XFEM Linear System:

$$\begin{bmatrix} A_{rr} & A_{rx} \\ A_{xr} & A_{xx} \end{bmatrix} \begin{bmatrix} u_r \\ u_x \end{bmatrix} = \begin{bmatrix} \tilde{f}_r \\ \tilde{f}_x \end{bmatrix}$$



nDOF = 5552
nnz = 101004

Standard SA-AMG for elastic problems performs poorly!