

# Algebraic Multigrid Techniques for the eXtended Finite Element Method

Axel Gerstenberger, Ray Tuminaro

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)

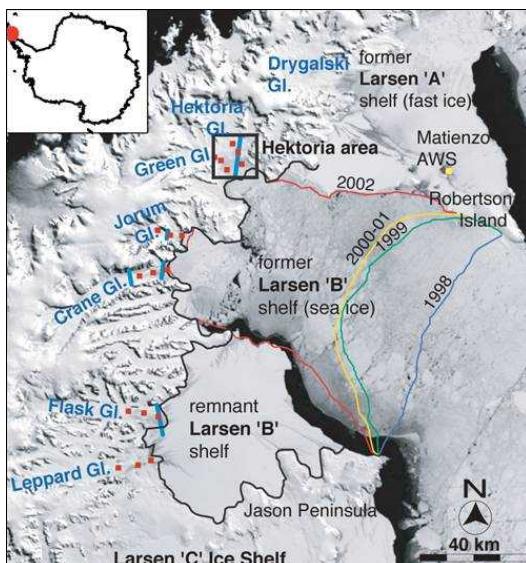
- allows to treat problems with singularities or discontinuities that are 'impractical' to be resolved by h-adaptivity. (*adapted from Wikipedia*)
- does so by extending the approximation space with known analytic solutions – similar to p-adaptivity, but not the same.
- has been applied to 3d
  - Crack 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.

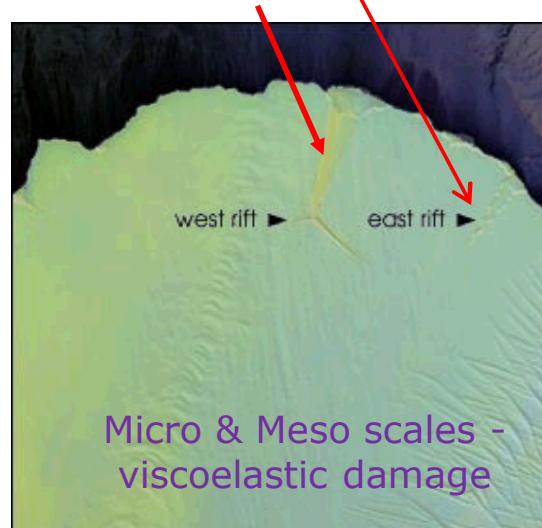
Ice shelves in Antarctica:



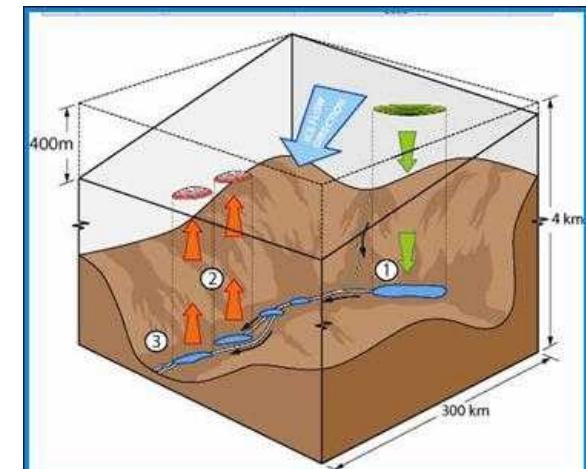
Larsen 'B' diminishing shelf  
1998-2002

Other example: Wilkins ice shelf 2008

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



Micro & Meso scales - viscoelastic damage

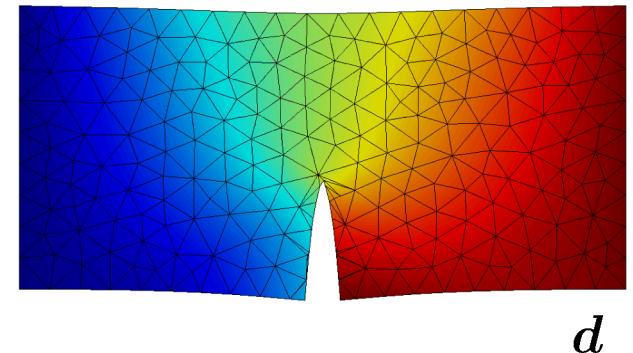


Glacial hydrology  
(Source: <http://www.sale.scar.org>)

# Computational Modeling of Fracture

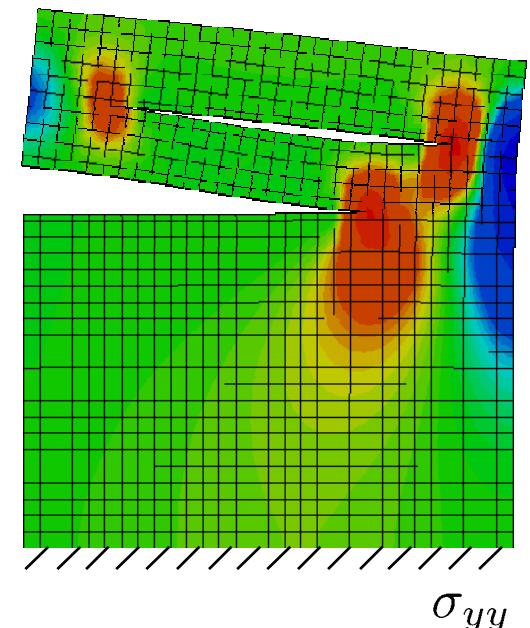
## Classical FEM approach to fracture mechanics

- 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



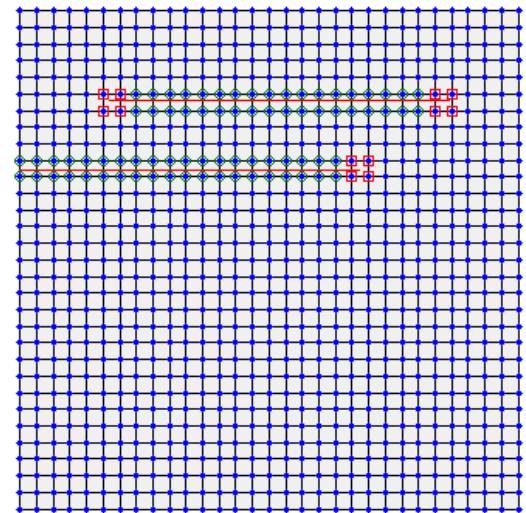
\* Belytschko & Black (1999), Moes et al. (1999)

# XFEM Formulation for Cracks

Displacement approximation (shifted basis form.)

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

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



- Jump Enrichment
- Tip Enrichment (brittle crack)

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

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

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

Global system

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

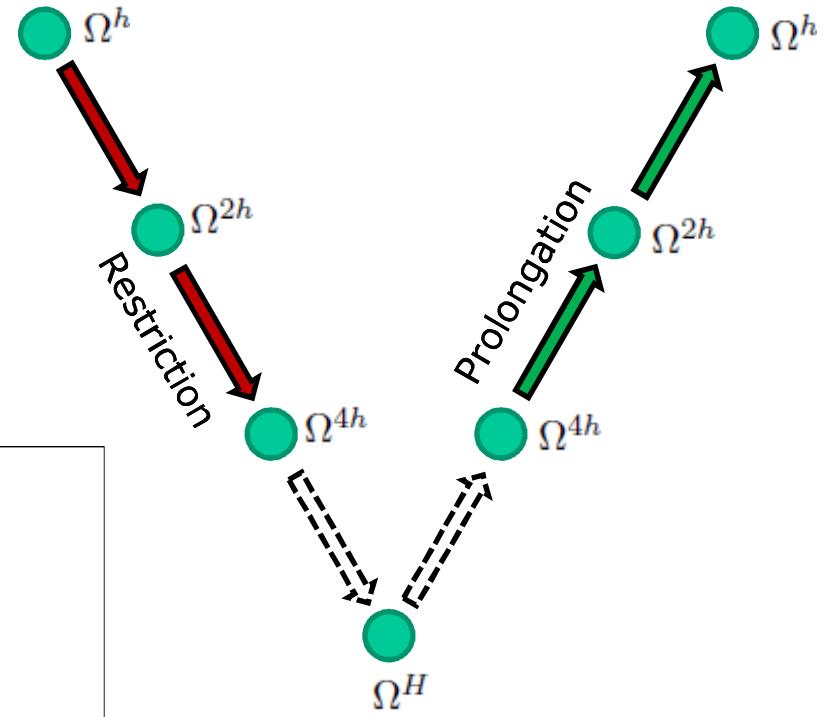
$$\mathbf{f} = \sum_e \int_{\Gamma_e} \mathbf{N}_e^T h \, d\mathbf{x} + \sum_e \int_{\Omega_e} \mathbf{N}_e^T \rho \, d\mathbf{x}$$

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

# 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

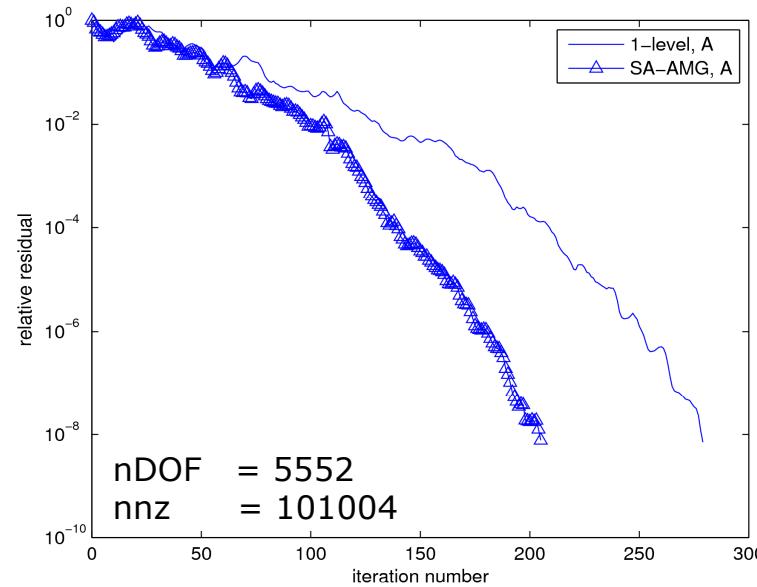
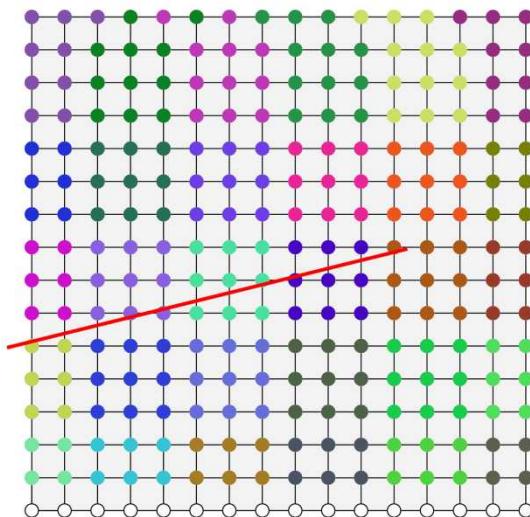
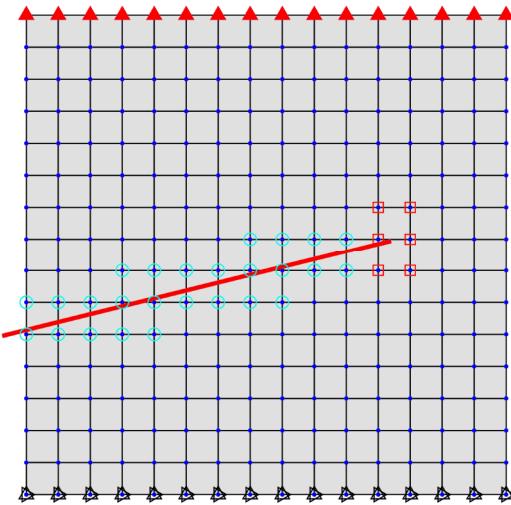
```
// Solve  $A^{[k]}u^{[k]} = b^{[k]}$ 
procedure multilevel( $b^{[k]}, u^{[k]}, k$ )
   $u^{[k]} = \mathcal{R}^{[k]}(A^{[k]}, b^{[k]}, u^{[k]})$ ;
  if ( $k \neq \ell$ )
     $r^{[k]} = b^{[k]} - A^{[k]}u^{[k]}$  ;
     $u^{[k+1]} = 0$ ;
     $u^{[k+1]} = \text{multilevel}((P^{[k]})^T r^{[k]}, u^{[k+1]},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



Direct solve at the coarsest level

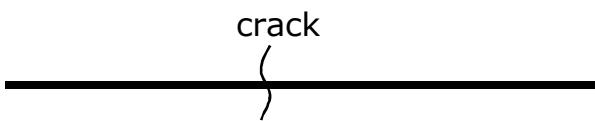
Recursive multigrid V Cycle consisting of  $l$  cycles to solve  $Au=b$

# 'Standard' SA-AMG for fracture problems

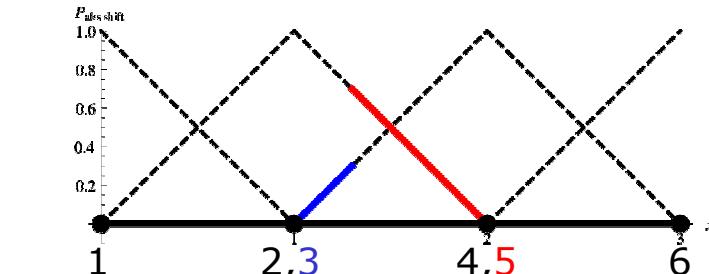


- Aggregation
  - Aggregates should not cross crack
- Nullspace
  - Elasticity: 3 ZEMs
  - Uncoupled domains: 6 ZEMs or more?
- Assumption of 2 unknowns per node fails
  - 2, 4, or 10 DOFs per node

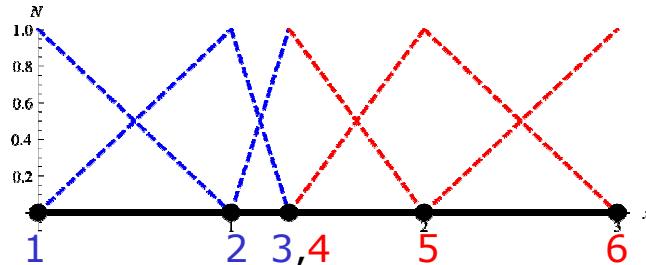
# Distinct region representation



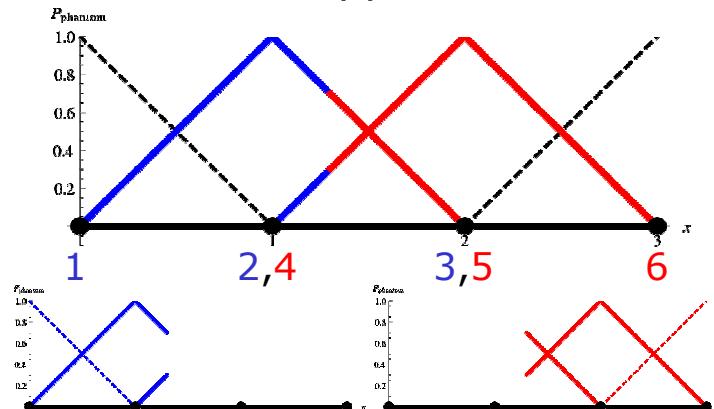
XFEM: modified shifted enrichment



FEM



Phantom node approach



$$K$$

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

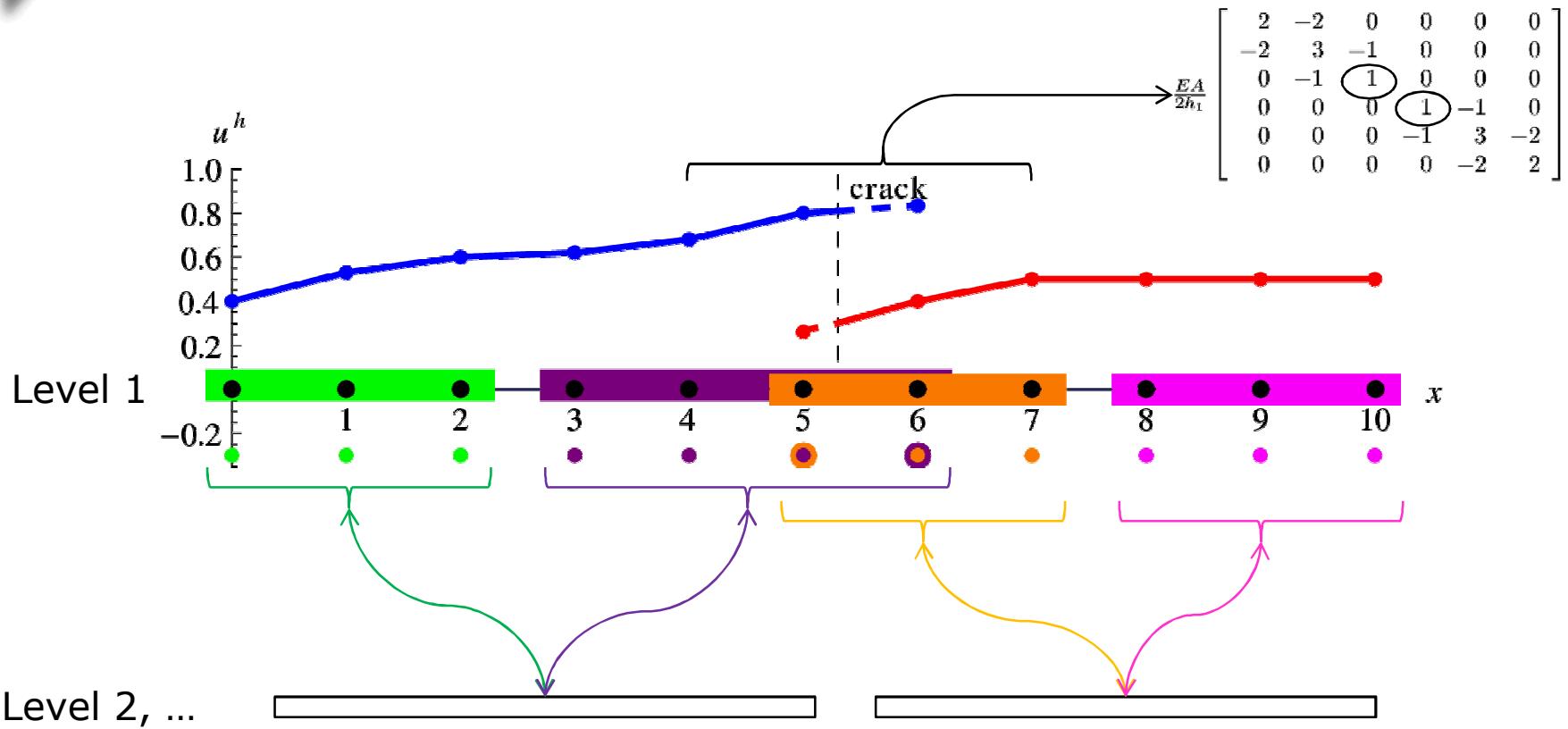
$$\frac{EA}{2h_1} \begin{bmatrix} 2 & -2 & 0 & 0 & 0 & 0 \\ -2 & 4 & 1 & -2 & -1 & 0 \\ 0 & 1 & 1 & -1 & 0 & 0 \\ 0 & -2 & -1 & 4 & 1 & -2 \\ 0 & -1 & 0 & 1 & 1 & 0 \\ 0 & 0 & 0 & -2 & 0 & 2 \end{bmatrix} \quad \frac{\rho Ah_1}{24} \begin{bmatrix} 8 & 4 & 0 & 0 & 0 & 0 \\ 4 & 16 & 1 & 4 & 2 & 0 \\ 0 & 1 & 1 & 2 & 0 & 0 \\ 0 & 4 & 2 & 16 & 1 & 4 \\ 0 & 2 & 0 & 1 & 1 & 0 \\ 0 & 0 & 0 & 4 & 0 & 8 \end{bmatrix}$$

$$\frac{EA}{2h_1} \begin{bmatrix} 2 & -2 & 0 & 0 & 0 & 0 \\ -2 & 6 & -4 & 0 & 0 & 0 \\ 0 & -4 & 4 & 0 & 0 & 0 \\ 0 & 0 & 0 & 4 & -4 & 0 \\ 0 & 0 & 0 & -4 & 6 & -2 \\ 0 & 0 & 0 & 0 & -2 & 2 \end{bmatrix} \quad \frac{\rho Ah_1}{24} \begin{bmatrix} 8 & 4 & 0 & 0 & 0 & 0 \\ 4 & 12 & 2 & 0 & 0 & 0 \\ 0 & 2 & 4 & 0 & 0 & 0 \\ 0 & 0 & 0 & 4 & 2 & 0 \\ 0 & 0 & 0 & 2 & 12 & 4 \\ 0 & 0 & 0 & 0 & 4 & 8 \end{bmatrix}$$

$$\frac{EA}{2h_1} \begin{bmatrix} 2 & -2 & 0 & 0 & 0 & 0 \\ -2 & 3 & -1 & 0 & 0 & 0 \\ 0 & -1 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & -1 & 0 \\ 0 & 0 & 0 & -1 & 3 & -2 \\ 0 & 0 & 0 & 0 & -2 & 2 \end{bmatrix} \quad \frac{\rho Ah_1}{24} \begin{bmatrix} 8 & 4 & 0 & 0 & 0 & 0 \\ 4 & 15 & 2 & 0 & 0 & 0 \\ 0 & 2 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 2 & 0 \\ 0 & 0 & 0 & 2 & 15 & 4 \\ 0 & 0 & 0 & 0 & 4 & 8 \end{bmatrix}$$

(reordered for visualization)

# Aggregation for phantom nodes: 1D



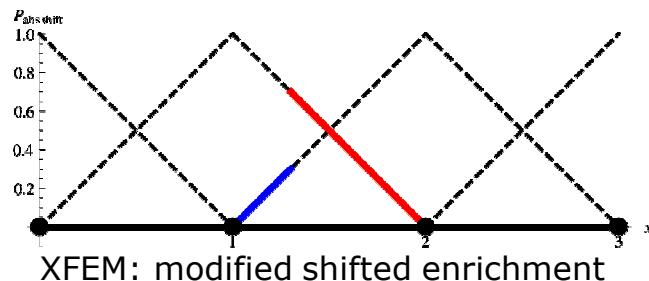
Aggregates seemingly overlap, but are **not** connected on any level!

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

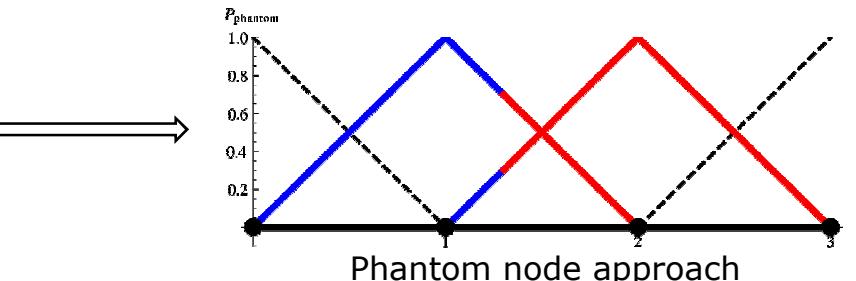
For each node  $I$  with jump DOFs:

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

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



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

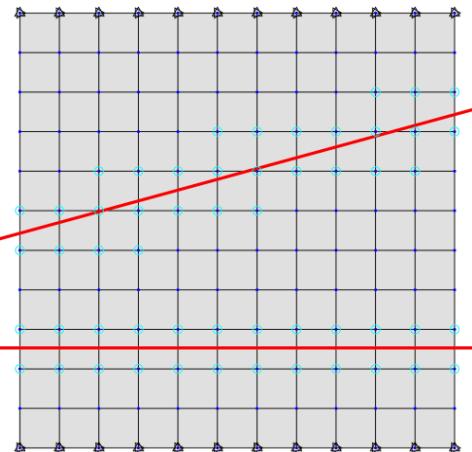


$\mathbf{G}$

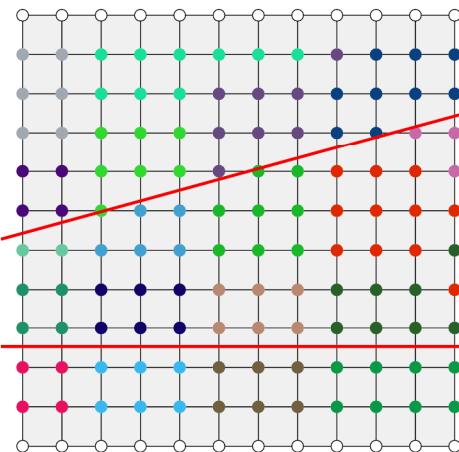
- is extremely sparse,
- is simple to produce,
- transformations are processor-local,
- applies only to jump DOFs
- exists for higher order Lagrange Polynomials and multiple dimensions

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

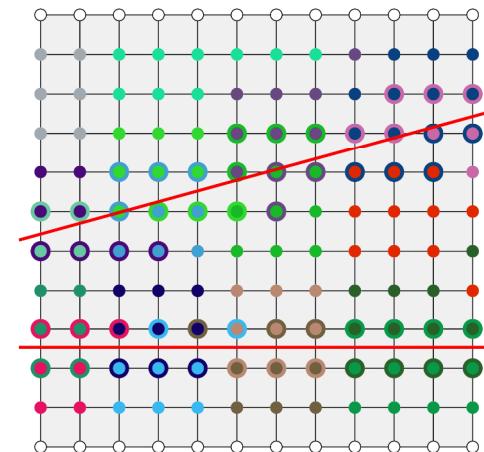
# Aggregation for phantom nodes: 2D



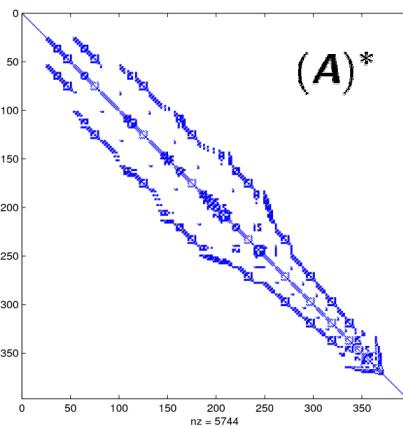
Mesh + Enrichment



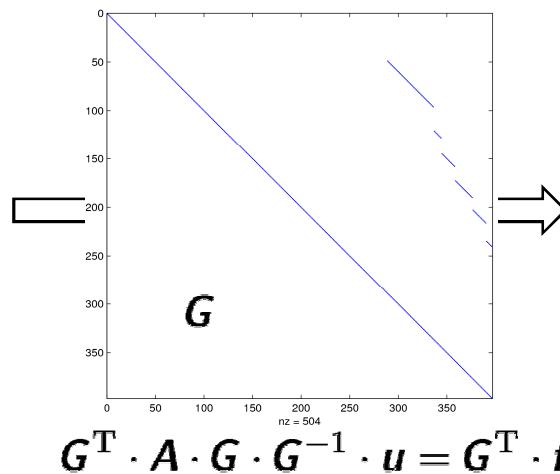
Standard DOFs only



Standard + Jump DOFs

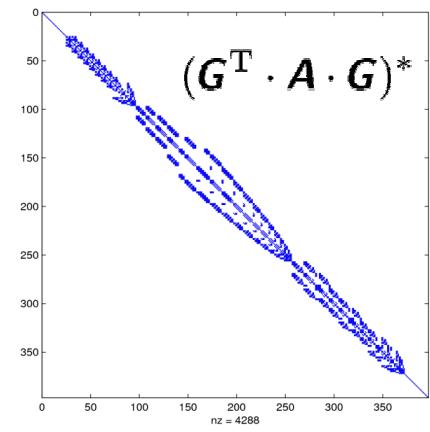


Modified shifted enrichment



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

$(\ )^*$  → sym. rev. Cuthill-McKee permutation

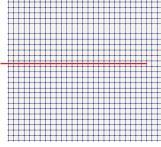
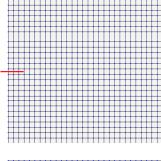
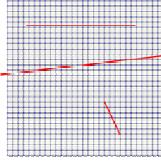
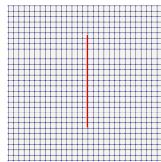
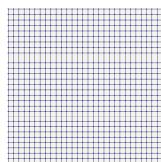


Phantom node approach

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

SA-OC: 1.28-1.40

# NullSpace for Jump & Tip Enrichments

2D Elasticity problem has 3 zero energy modes

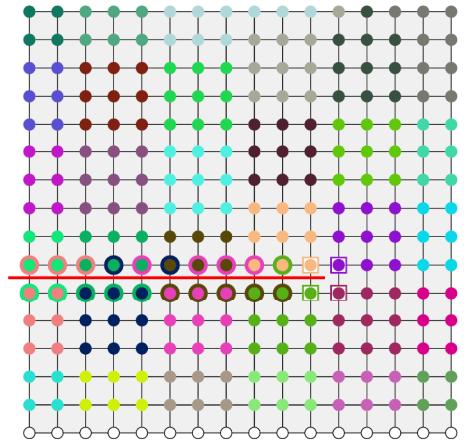
	1	2	3
Dx_I	1	0	-y_I
Dy_I	0	1	x_I
	...		...

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

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

- Don't transform tip dofs!



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

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

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

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

- Pre-smoother:

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

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

- Post-smoother

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

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

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

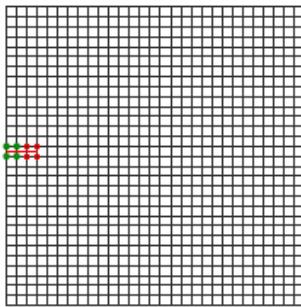
# Numerical Results...

## Test Cases:

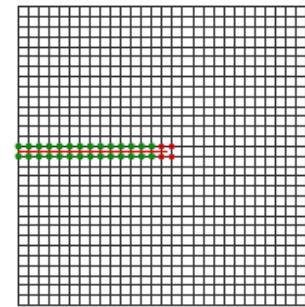
- Both edge cracks and interior cracks considered
- CG preconditioned with AMG

- 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

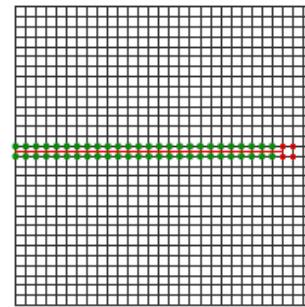
### Single Propagating Crack



(a) Case 1a

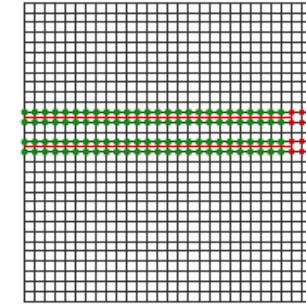


(b) Case 1b

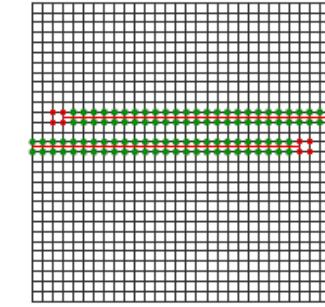


(c) Case 1c

### Two Cracks

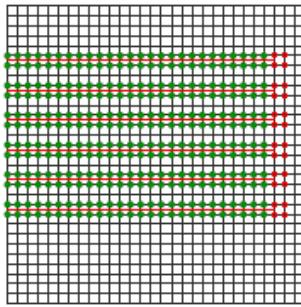


(d) Case 2a

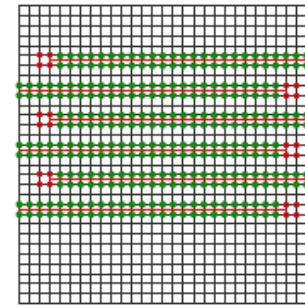


(e) Case 2b

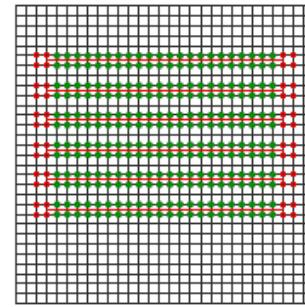
### Six Cracks



(f) Case 3a

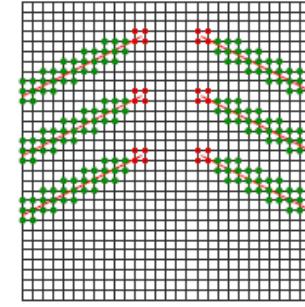


(g) Case 3b

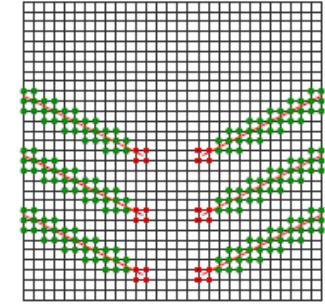


(h) Case 4

### Inclined Cracks



(i) Case 5a



(j) Case 5b

# Numerical Results for full XFEM system

Without cracks



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

SA-OC: 1.28-1.40

EM-OC: 1.13-1.17

# Numerical Results for full XFEM system

Case	$n_e \times n_e$	$n_{\text{iter}}$								$\alpha_{\text{cond.}}$	
		1L		ML		ML, MS		ML, 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	

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

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?

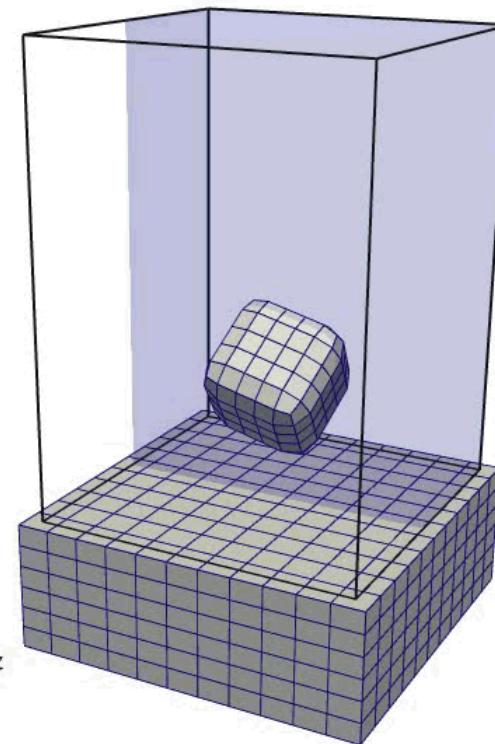
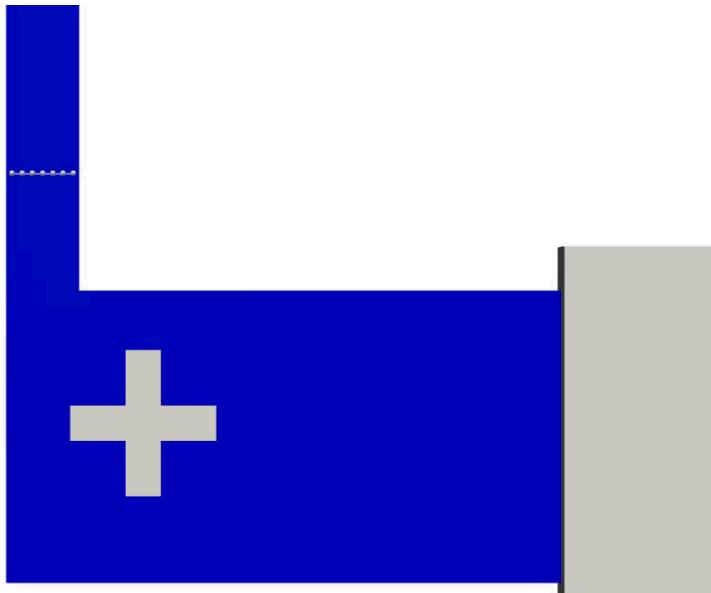
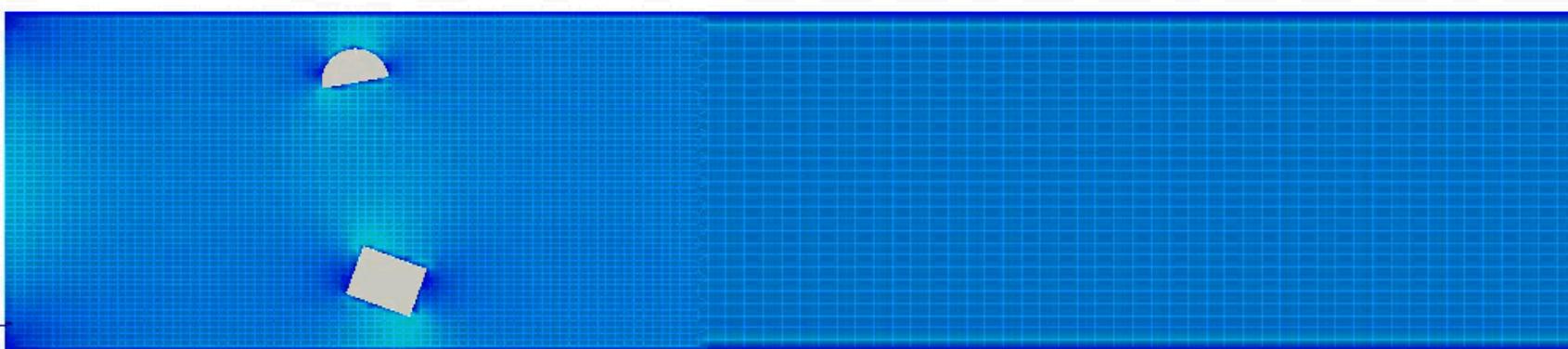


# Backup slides

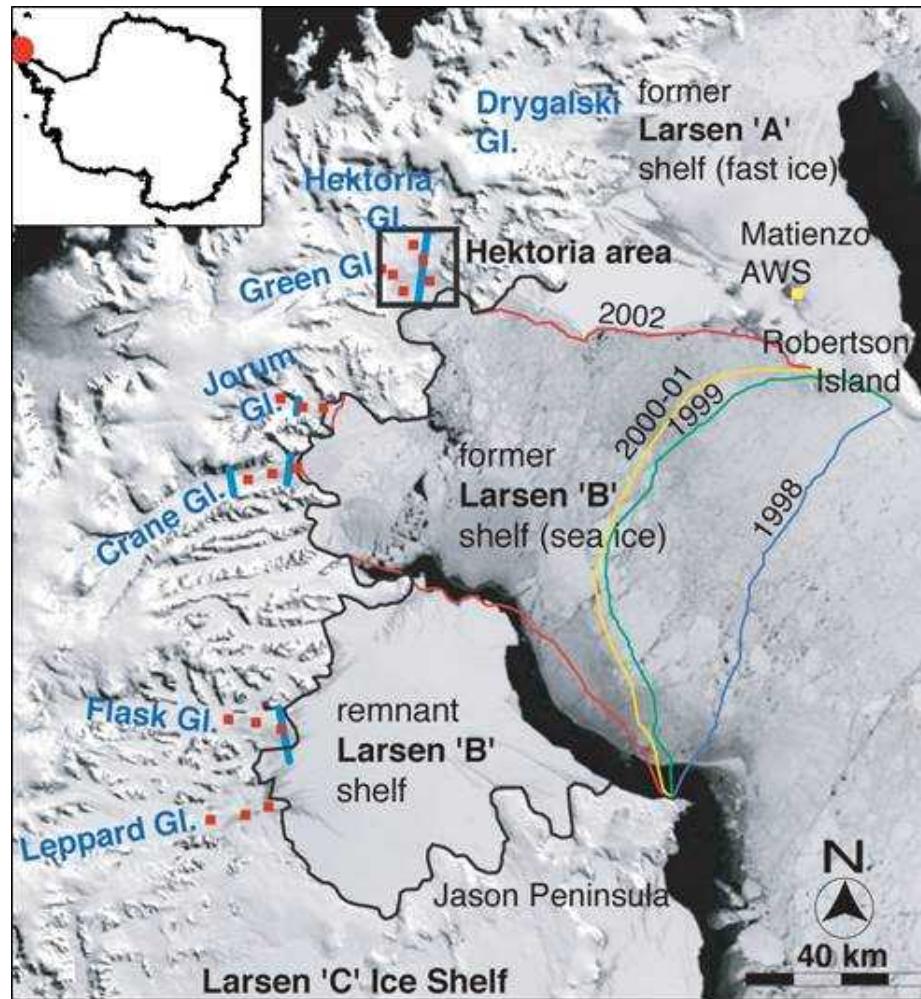


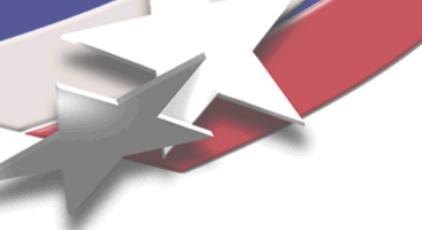
# XFEM flow and fluid-structure interaction

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

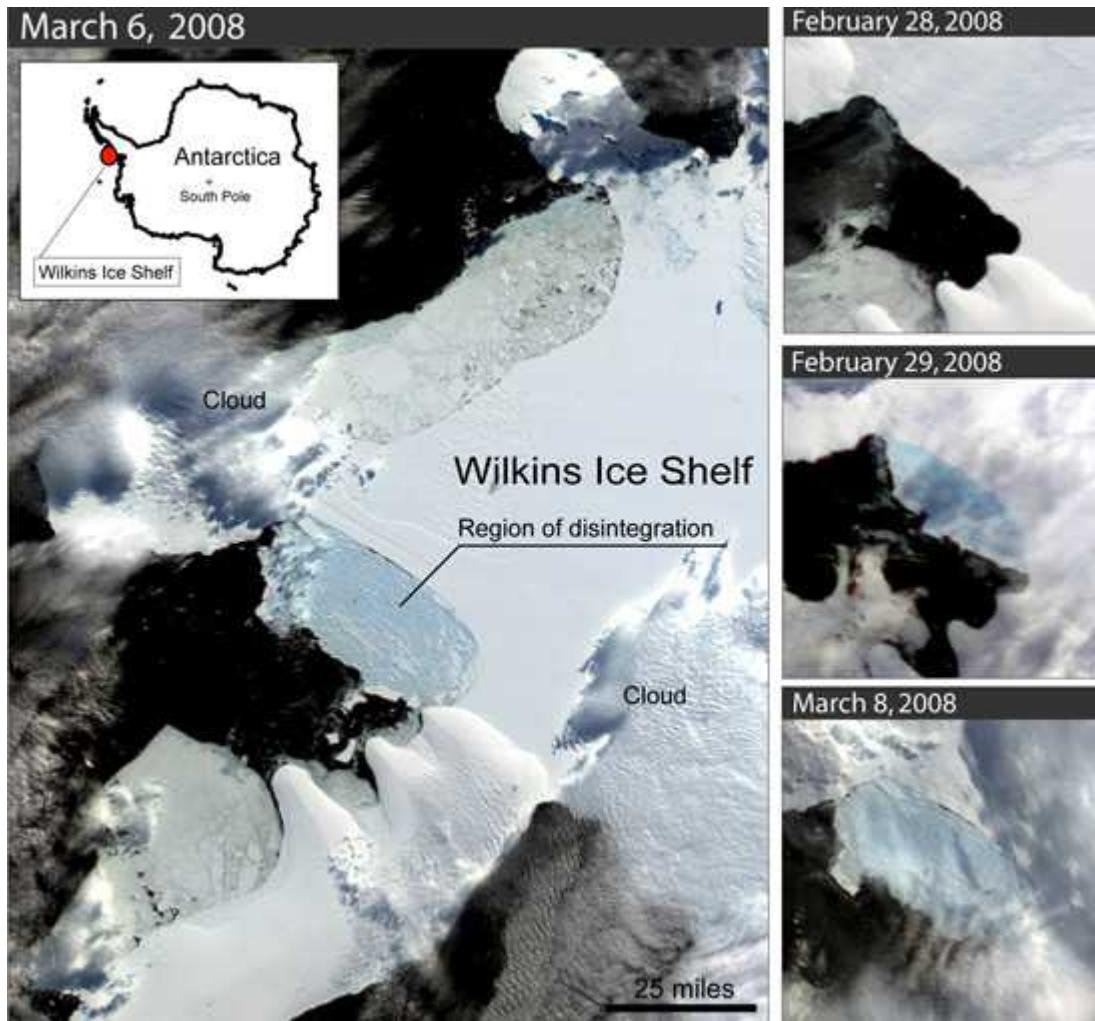


# Larsen 'B' shelf, 1998-2002





# Wilkins ice shelf, 2008



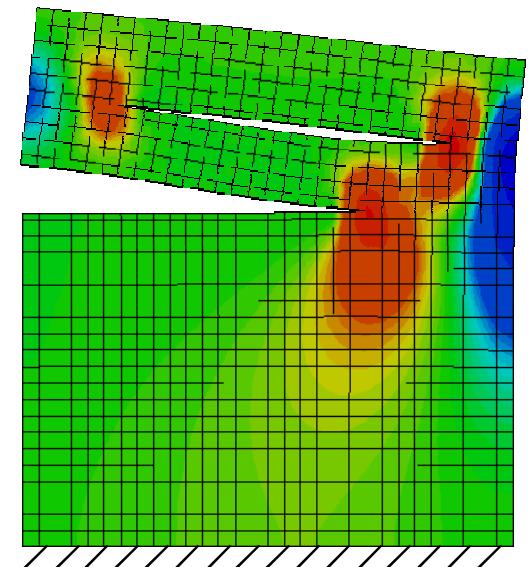
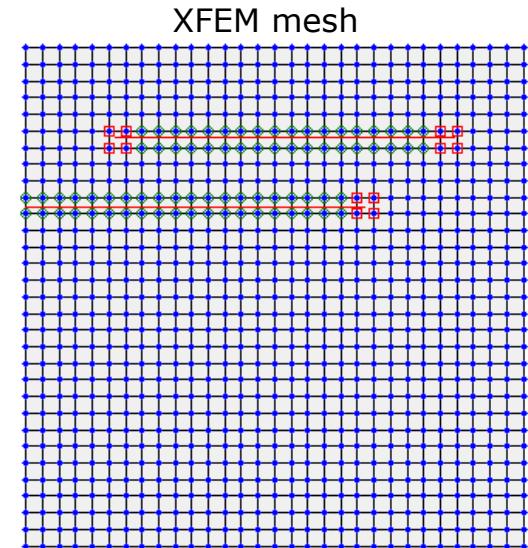
# Computational Modeling of Fracture

## 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



\* 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:

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

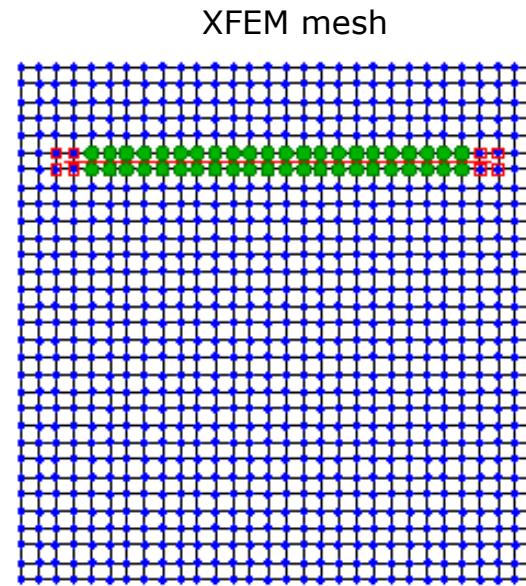
- Numerical quadrature for stiffness matrix

Assembly

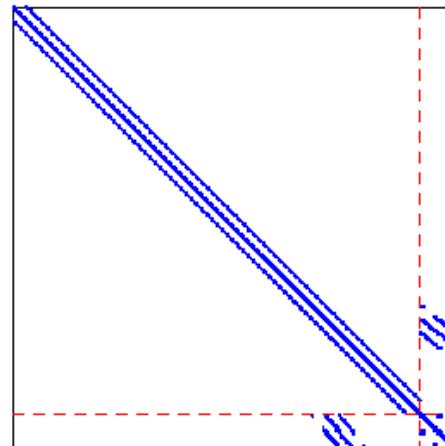
XFEM Linear System:

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

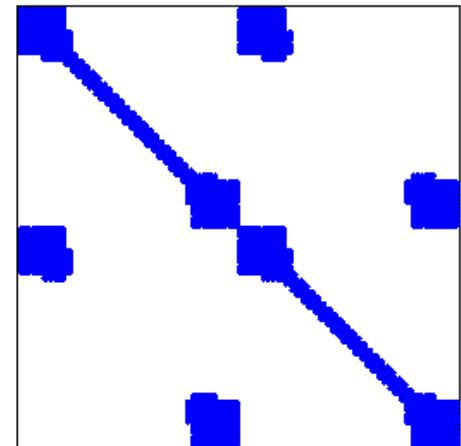
- Enriched DOF grouped together at the end in  $u_x$
- $A_{xx}$  small compared to  $A_{rr}$  for relatively small number of cracks



Sparsity pattern of  $\mathbf{A}$



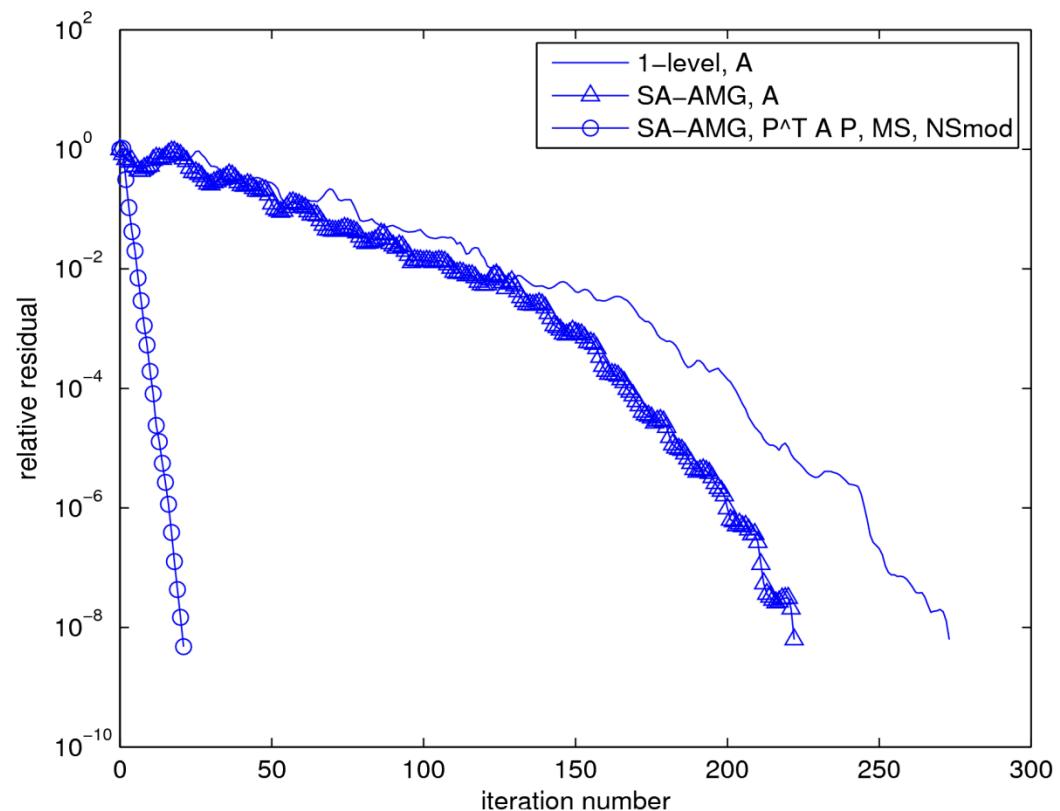
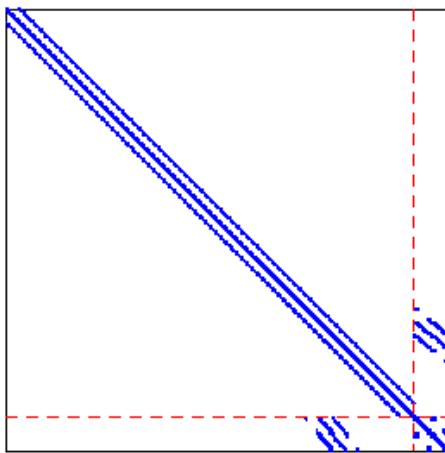
Sparsity pattern of  $\mathbf{A}_{xx}$



# '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!