Software Design for Non-conforming Finite Elements

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Computational and Applied Mathematics
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Earth Science and Engineering
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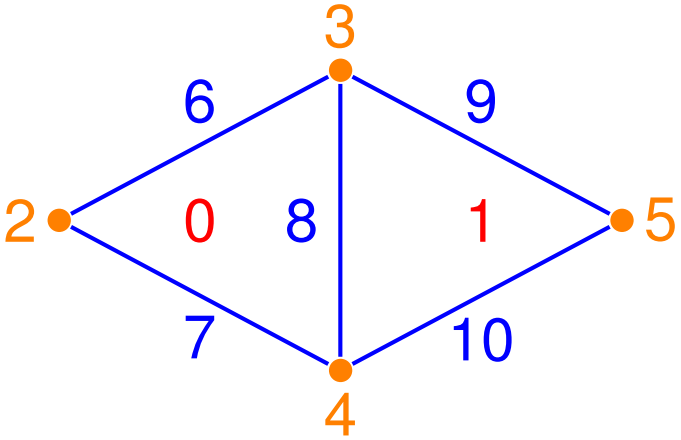
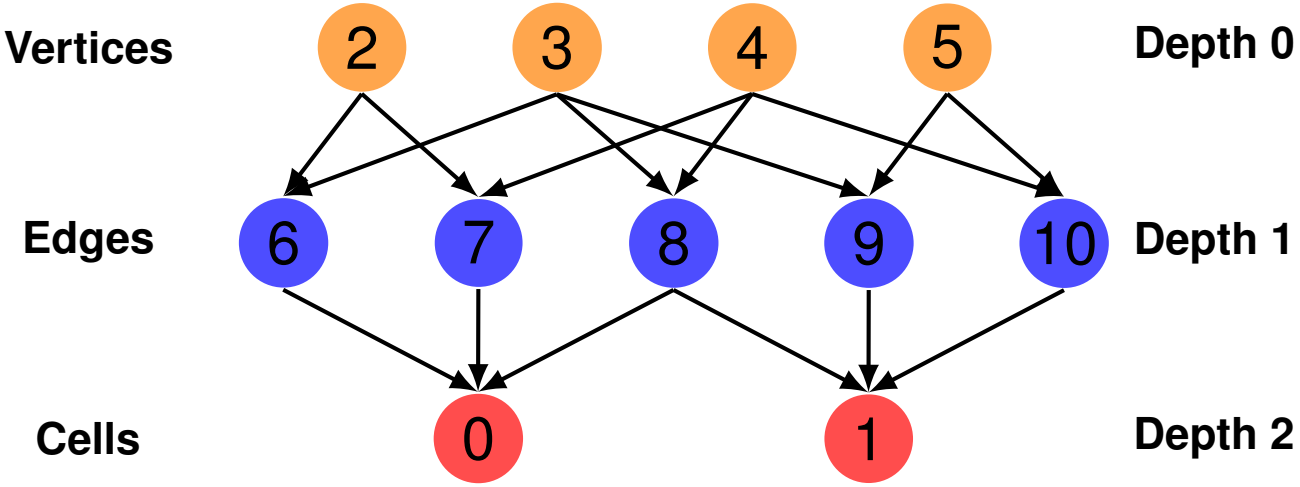
Main Point

We support structured AMR with an unstructured interface efficiently.

https://arxiv.org/abs/1508.02470

Sample Meshes
Interpolated triangular mesh





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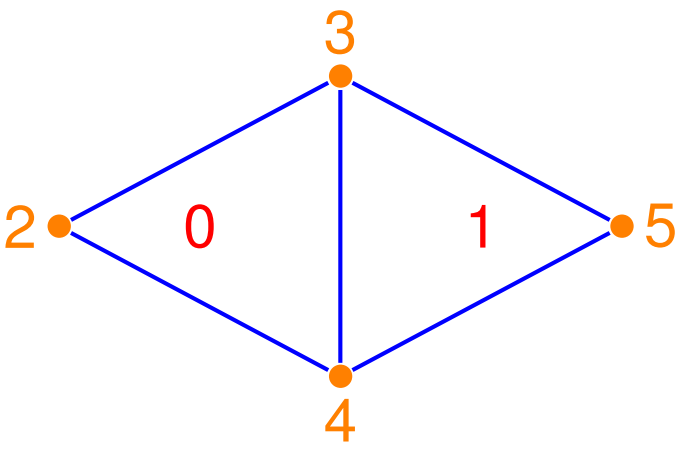
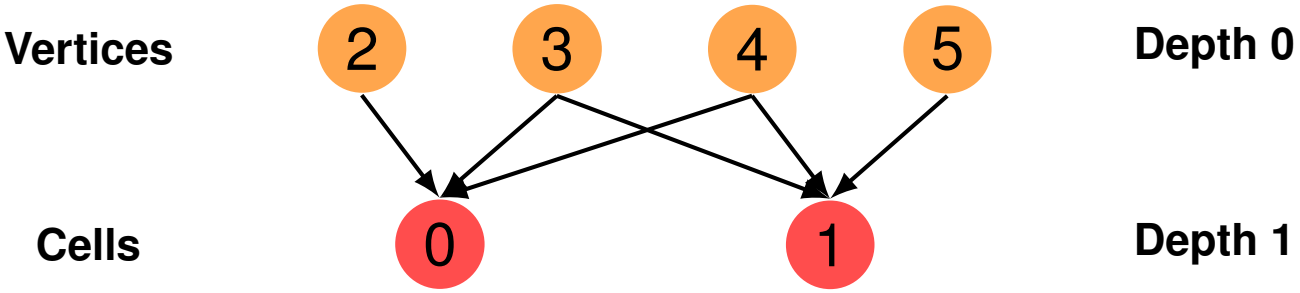
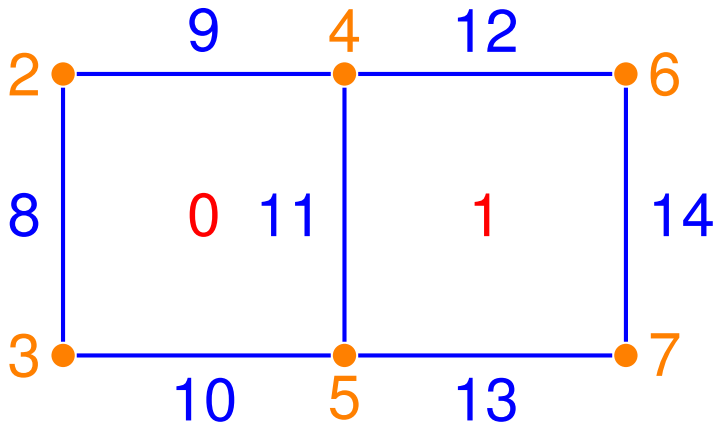
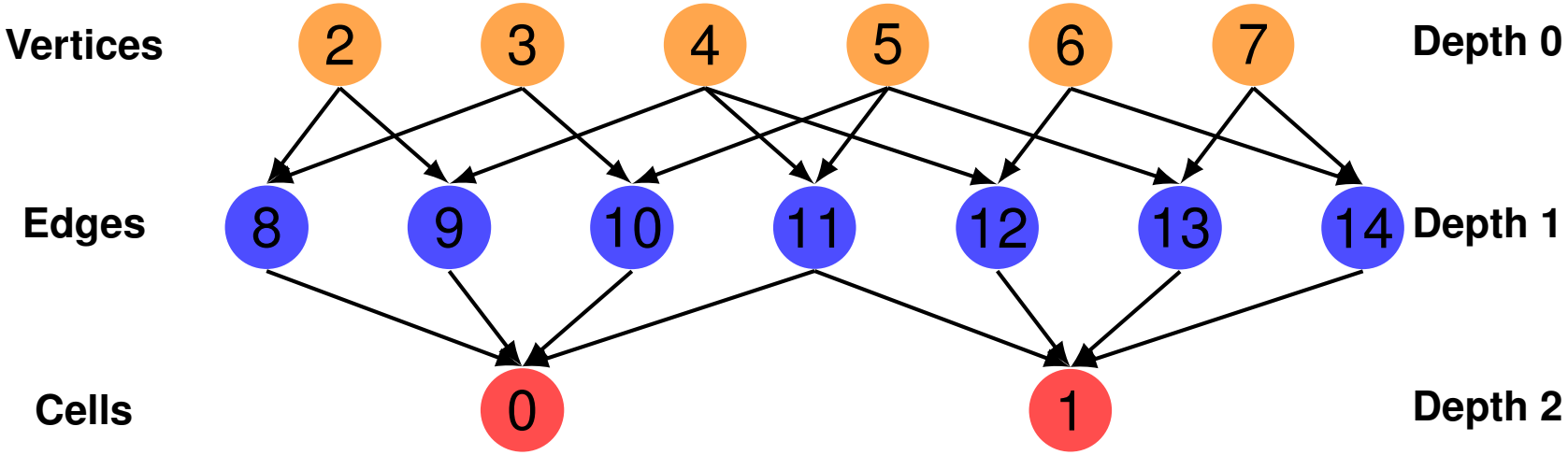




Sample Meshes
Interpolated quadrilateral mesh





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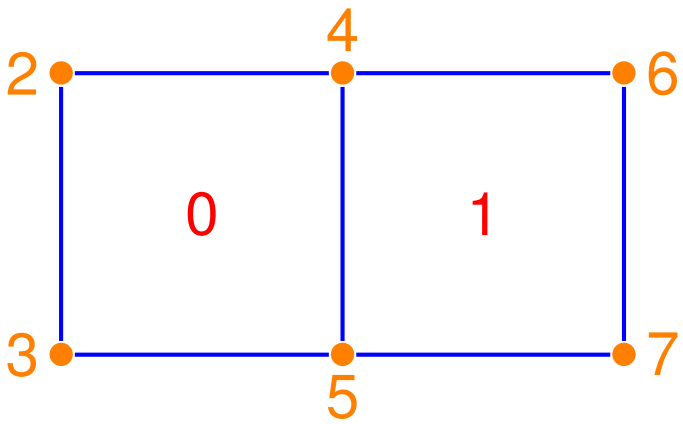
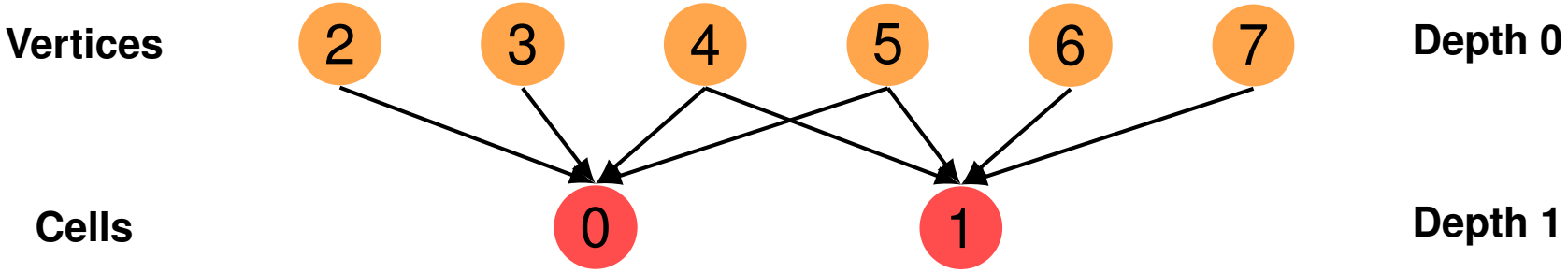
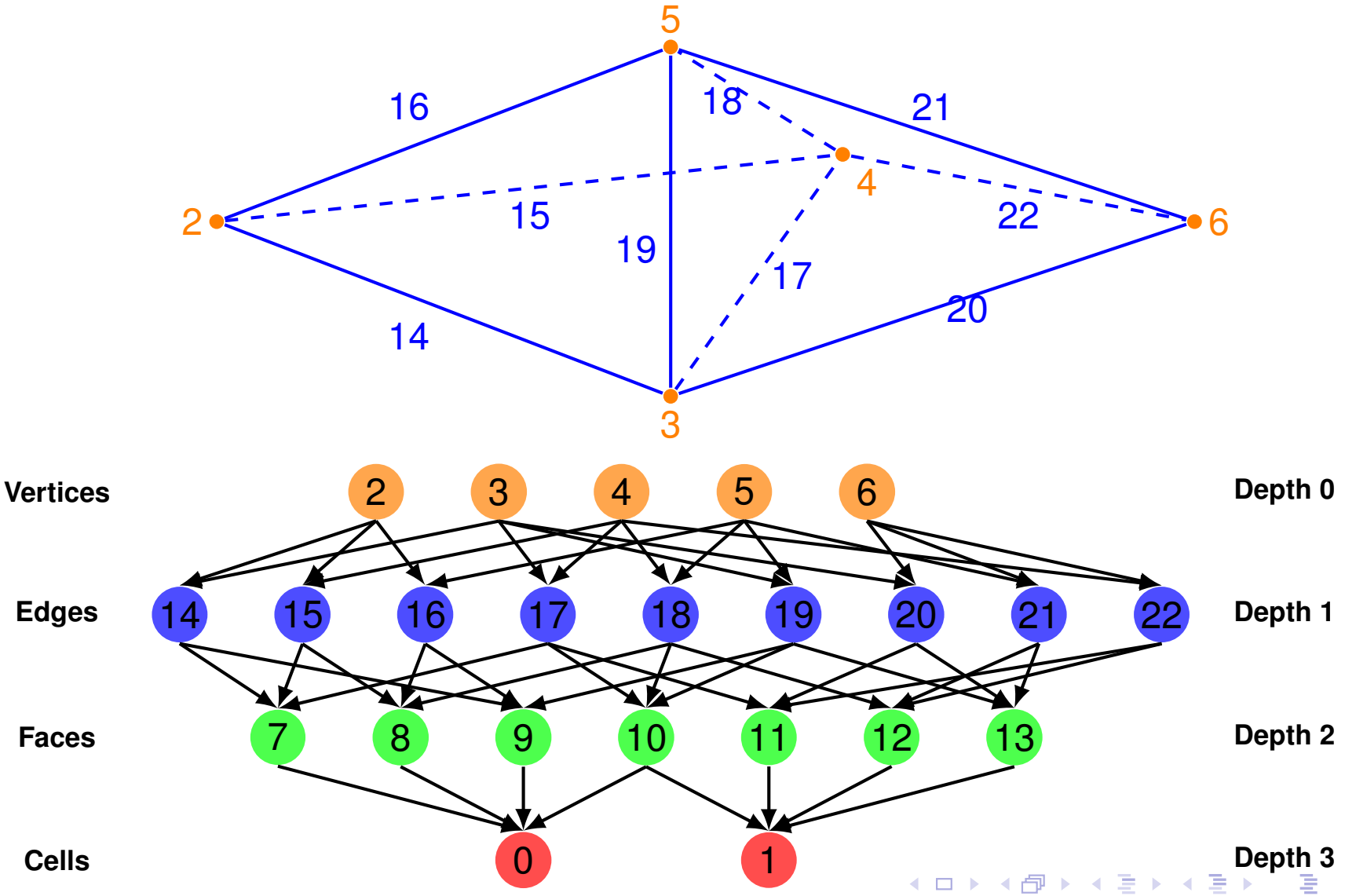


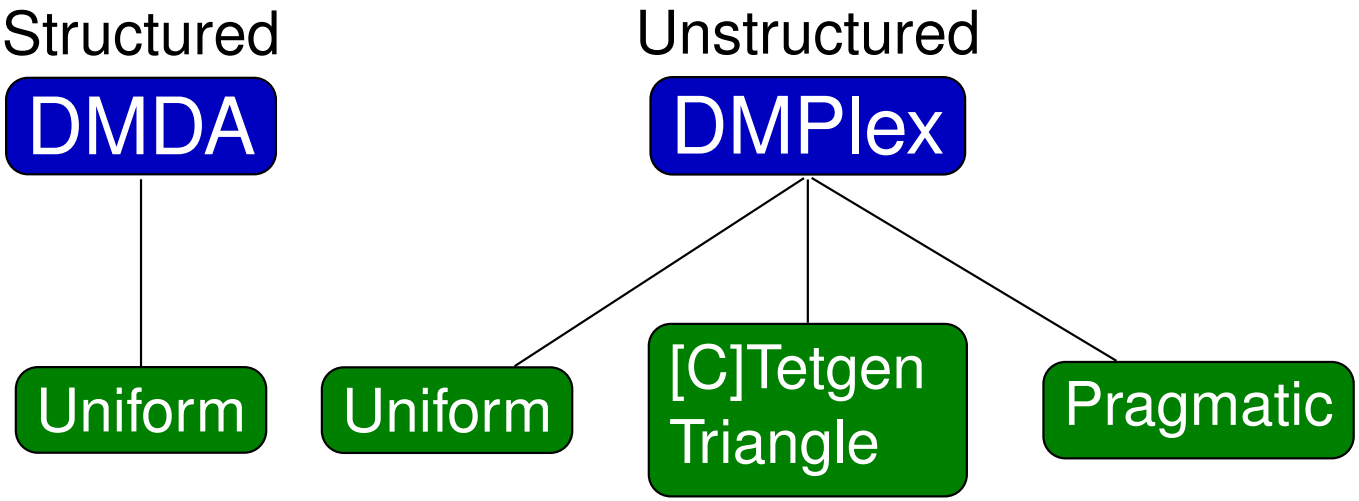


Sample Meshes

Interpolated tetrahedral mesh



Mesh Refinement in PETSc



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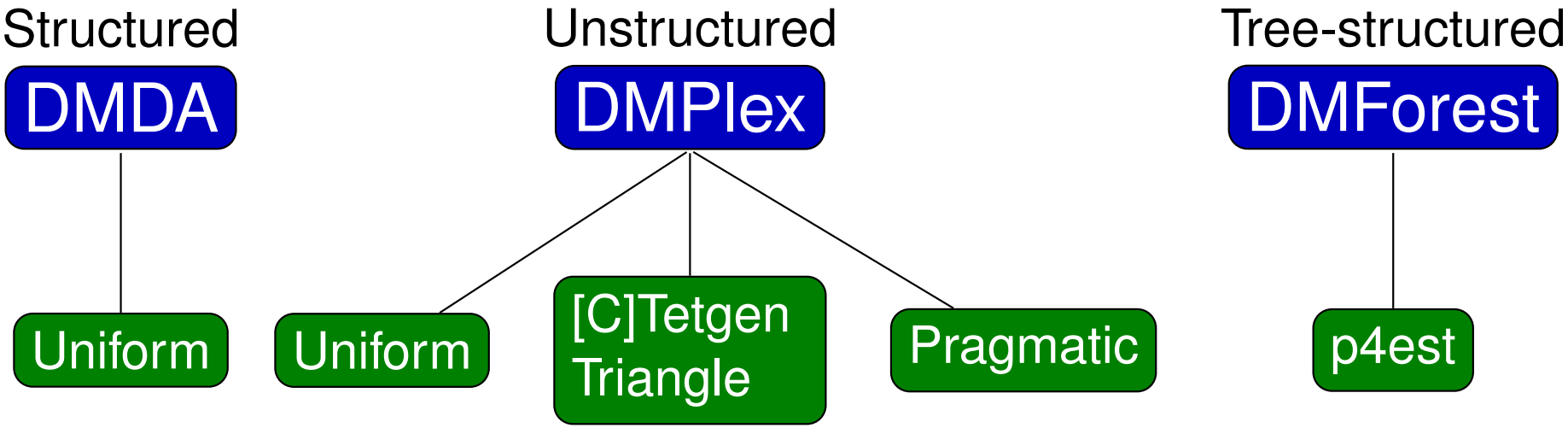
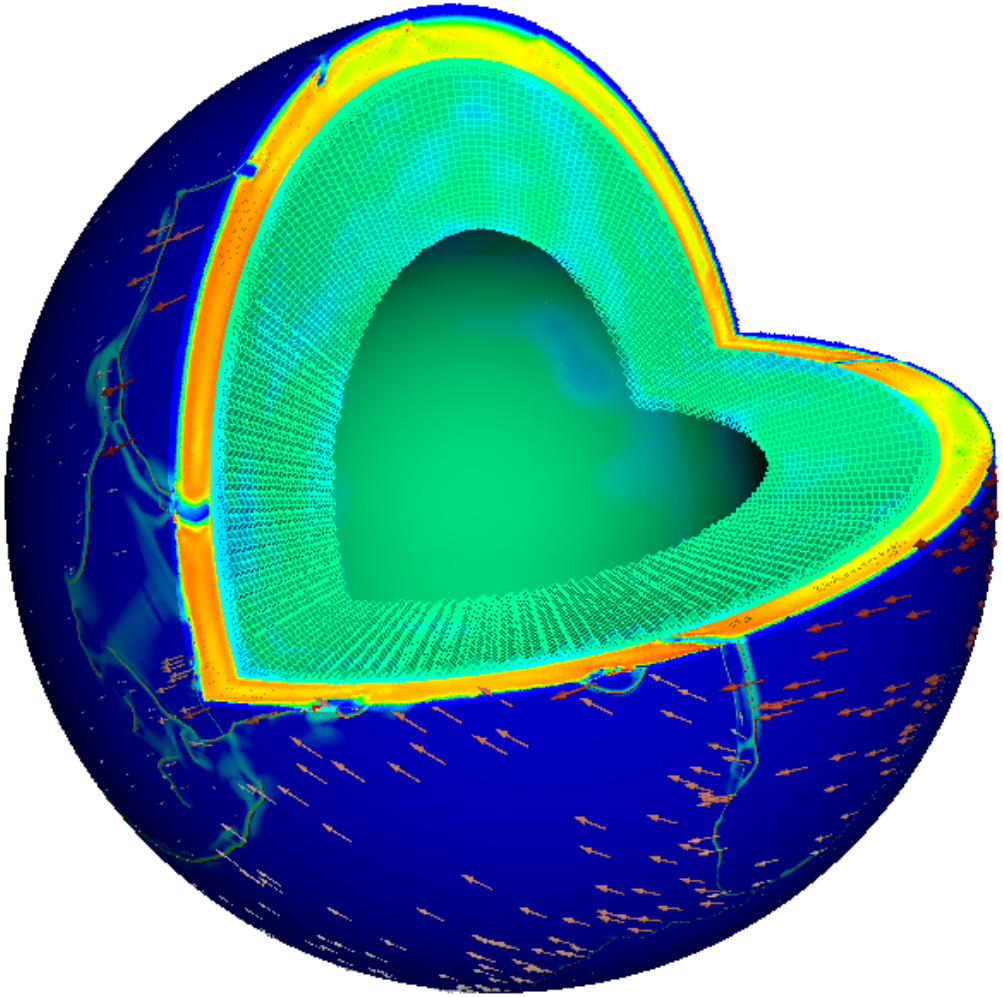


p4est overview

The p4est library (Carsten Burstedde and Toby Isaac) provides scalable AMR routines via a forest-of-octrees/quadtrees:

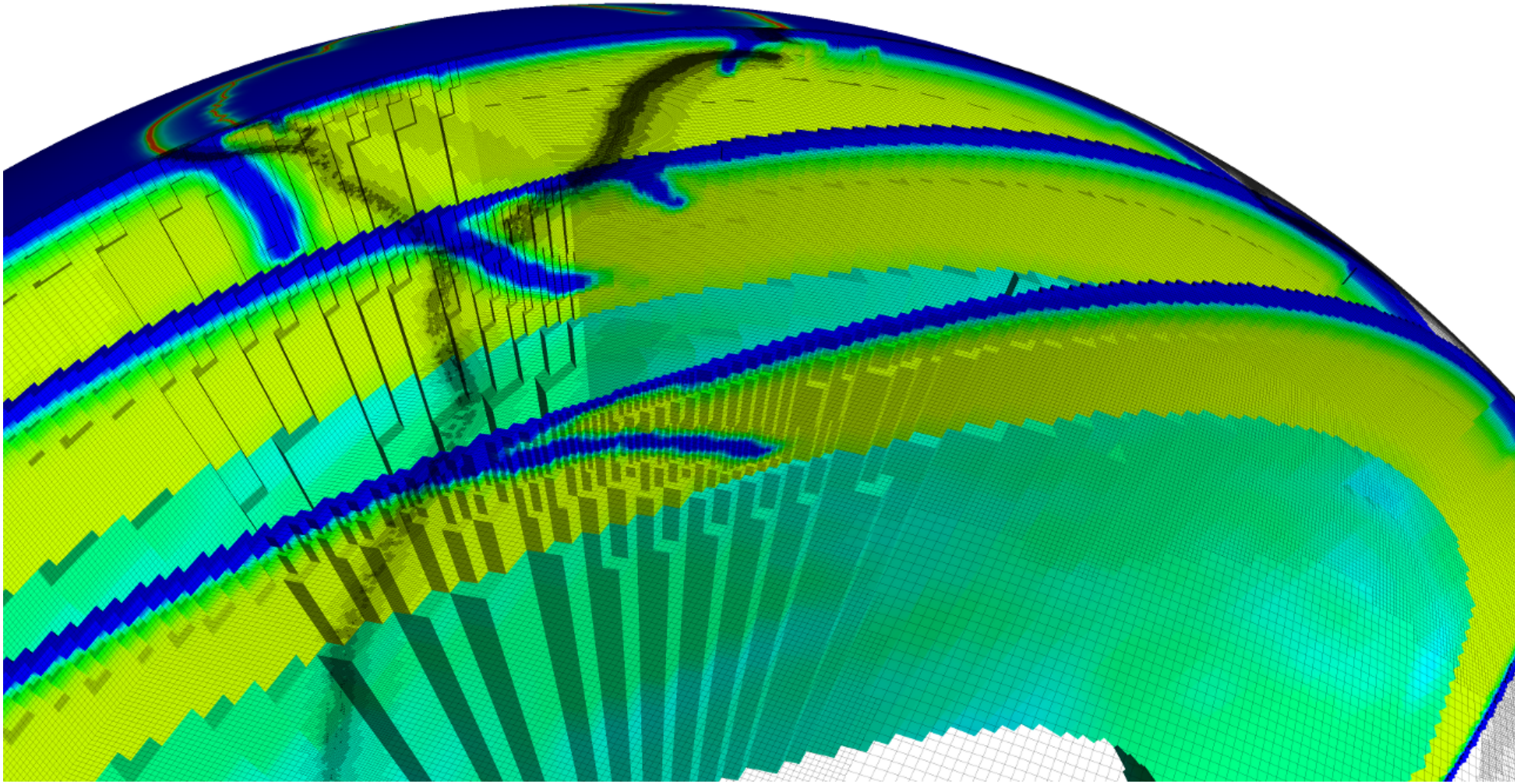
- a unstructured hexahedral mesh ("the forest");
- where each hexahedron contains an arbitrarily refined octree;
- space-filling curve (SFC) orders elements;
- philosophy: as-simple-as-possible coarse mesh describes geometry, refinement captures all detail.
- not a framework: does not have numerical methods
  - Used for parallelism by Deal.II
  - Tight integration with solvers (e.g., multilevel) is still the domain of experts (next slide)

p4est in geophysics



(Rudi et al., 2015), “An extreme-scale implicit solver for complex PDEs: highly heterogeneous flow in earth’s mantle,” doi:10.1145/2807591.2807675.

p4est in geophysics



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Outline

FEM Axioms

Three FEM axioms allow an element to be
computable in our framework,
meaning we can form
a global nodal basis W for the dual space V_h^*.

- Sparsity
- Matching
- Independence

Notation

P	Reference approximation (primal) space
Q	Reference measurement (dual) space
T	Reference Cell
S	Reference complex for T
P_i	Primal space on cell T_i
Q_i	Dual space on cell T_i

I. Sparsity

For each $\sigma_j \in Q$ there exists a point $p \in S$ such that,
if $\psi_k \in P(T)$ is σ_k's shape function,
meaning $\sigma_j(\psi_k) = \delta_{jk}$,
then $\mathrm{supp}(\psi_k) = \bigcup \mathrm{star}(p)$.

- Dual basis functions are *attached* to points in S
- Topological support describes function support
- Allows for compactly supported basis functions

Notation

φ_i^*	Pullback of T_i onto T, for H_1 $\varphi_i^* f = f \circ \varphi_i$
$\varphi_{*,i}$	Pushforward of T onto T_i, the adjoint of φ_i^*
$P(X)$	Trace space of $P(T)$ on $X \subset \overline{T}$

II. Matching

$$\text{If } \mathcal{F} := \overline{T_i} \cap \overline{T_j} \neq \emptyset, \text{ then}$$
$$\psi \in P(\varphi_j^{-1}\mathcal{F}) \Rightarrow \varphi_i^* \varphi_j^{-*}\psi \in P(\varphi_i^{-1}\mathcal{F})$$

- Traces of primal spaces for adjacent cells "line up"
- Can pullback or pushfoward to F from either side

For H_1, we have

$$\begin{aligned} \varphi_i^* \varphi_j^{-*}\psi &\in P(\varphi_i^{-1}\mathcal{F}) \\ \varphi_j^{-*}\psi &\in P(\mathcal{F}) \\ \psi &\in P(\varphi_j^{-1}\mathcal{F}) \end{aligned}$$

Notation

Q^p	Reference functionals associated with $p \in S$, so that $Q = \bigcup_{p \in S} Q^p$
Q_i^p	Pushforward of functionals to cell T_i, $\varphi_{i*} Q^p$, so that $Q_i = \bigcup_{p \in Q} Q_i^p$
Sym_N	The symmetric group on N elements

III. Independence

If $\exists p, q \in S$ such that $\varphi_i(p) = \varphi_j(q)$
for adjacent cells T_i and T_j,
then $\exists M \in \mathrm{Sym}$ such that $\mathcal{Q}_i^p = M\mathcal{Q}_j^q$.

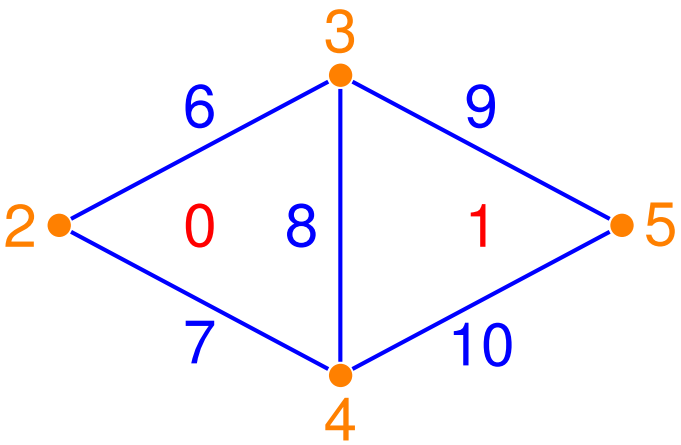
- Traces of dual spaces for adjacent cells "line up"
- Mappings push functionals forward into each other
- M encodes symmetries of polytopes in S

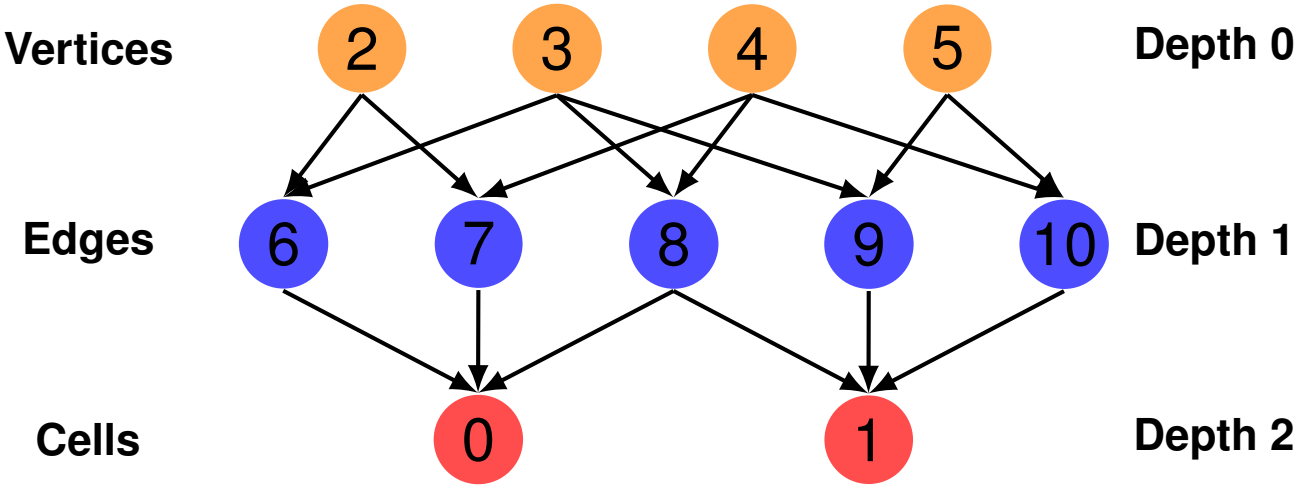
Outline

Outline

Sample Meshes

Interpolated triangular mesh





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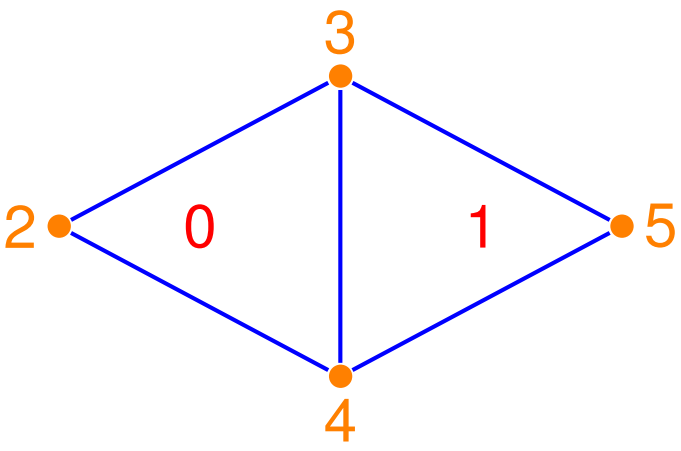
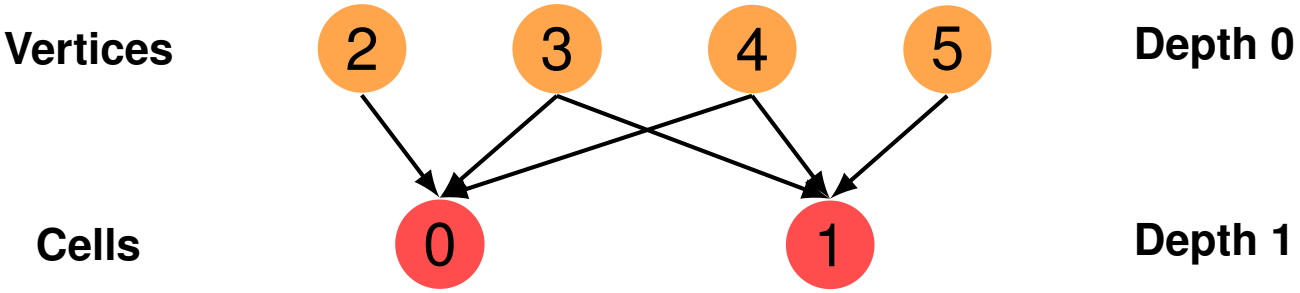
Optimized triangular mesh





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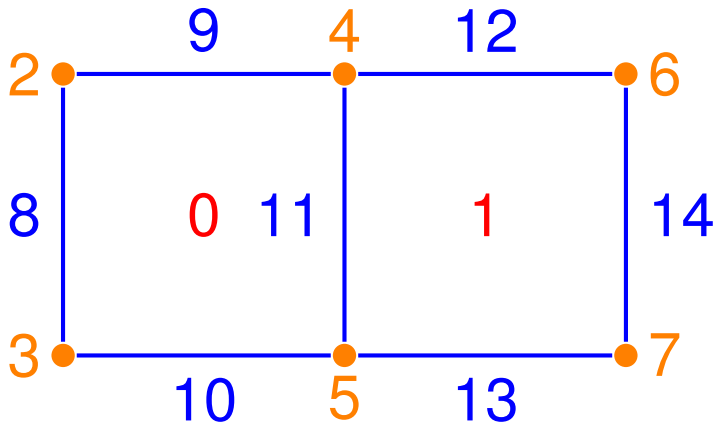
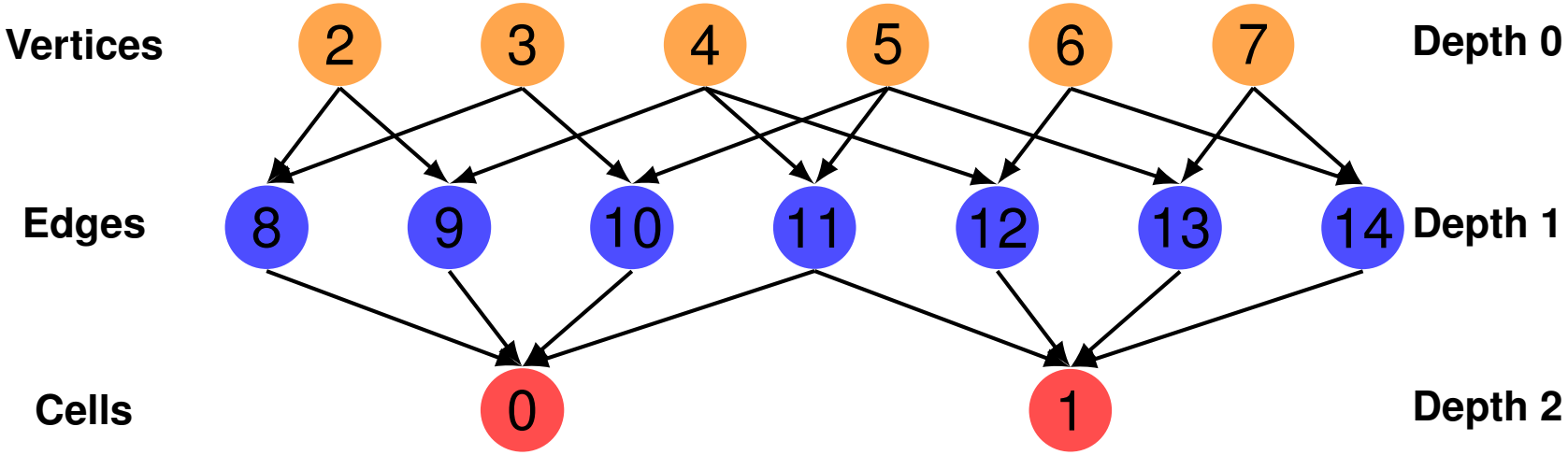
Interpolated quadrilateral mesh





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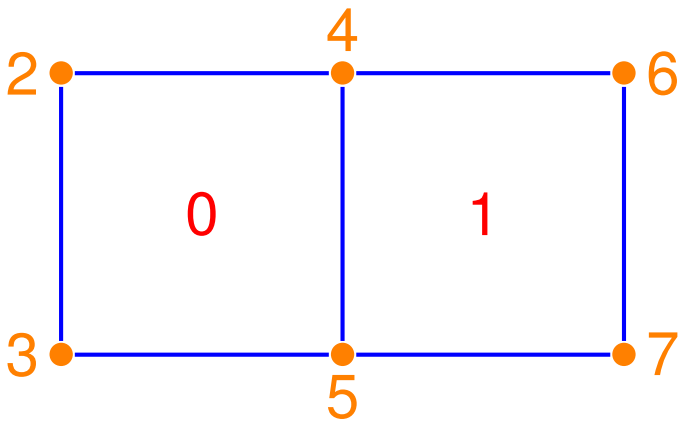

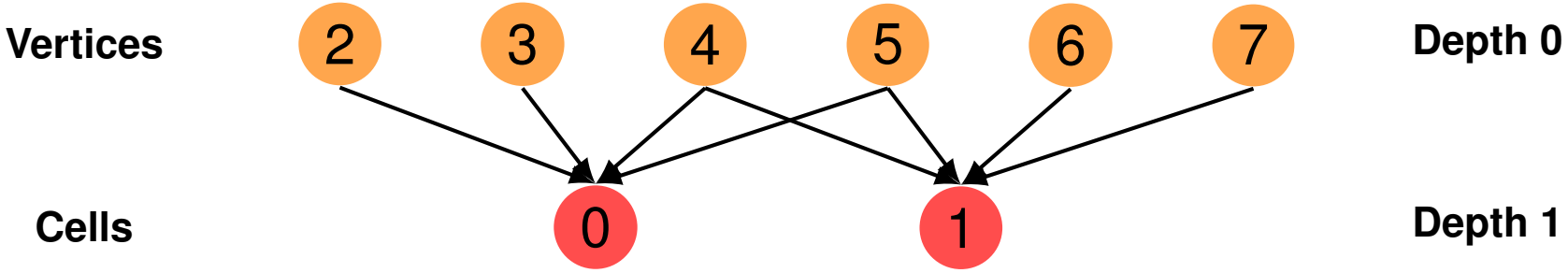

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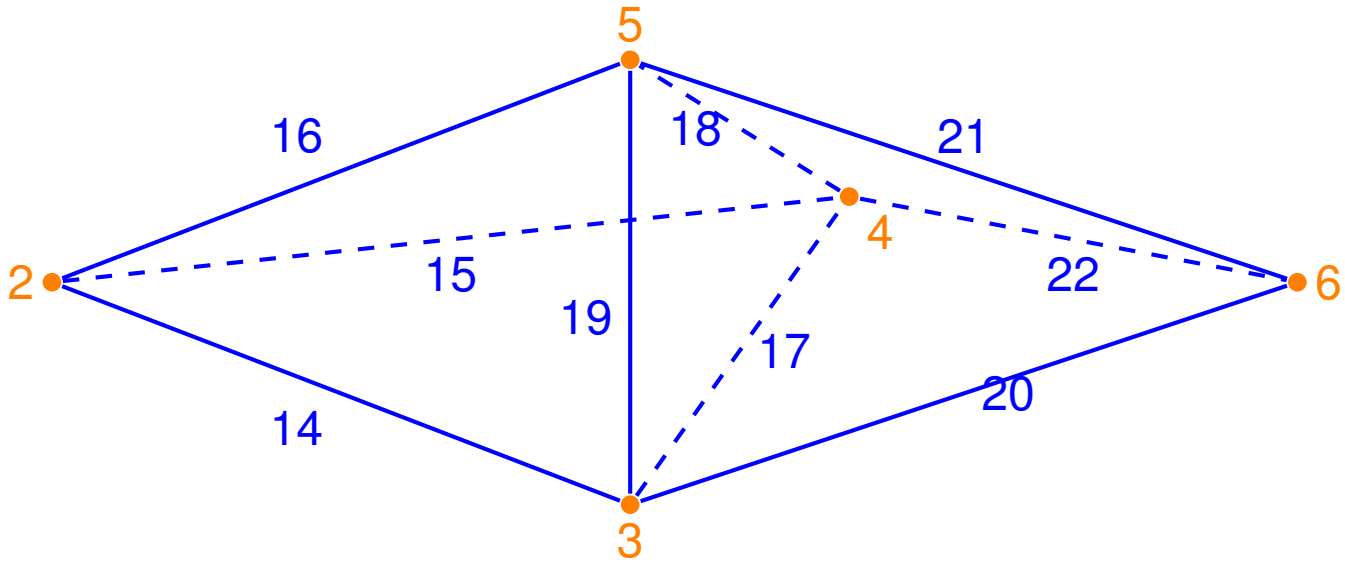
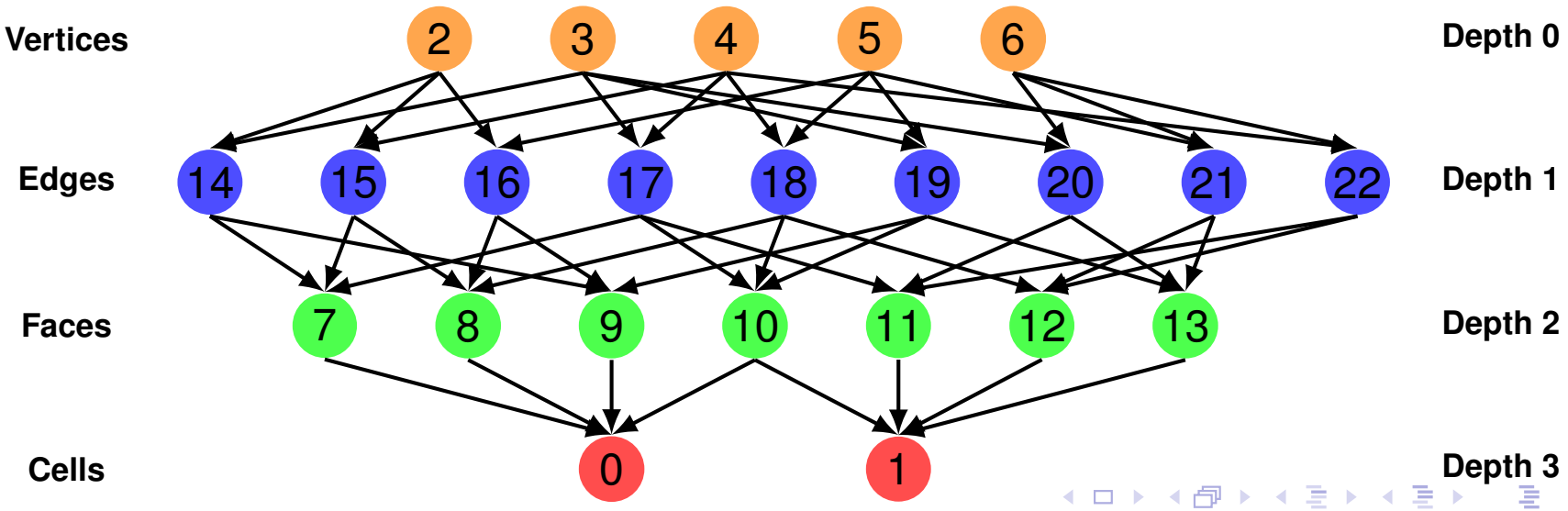
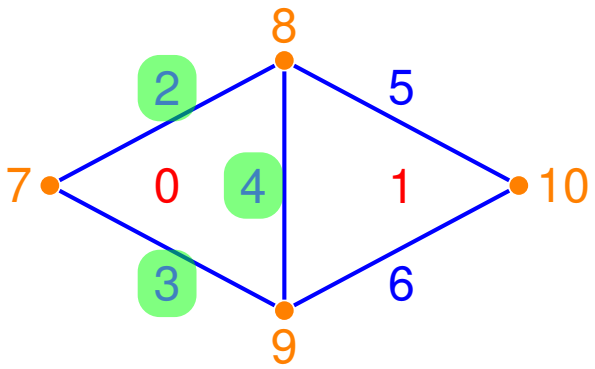


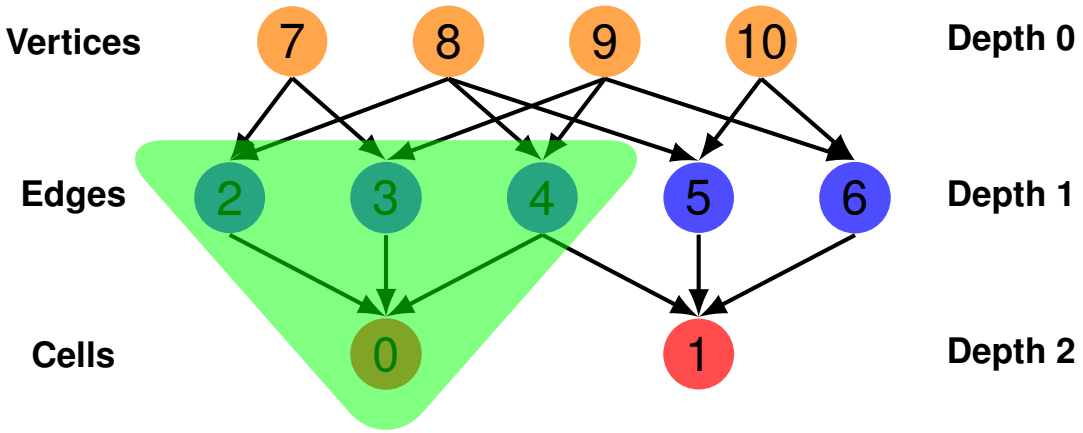


Basic Operations
Cone

We begin with the basic covering relation,

cone(0) = {2, 3, 4}

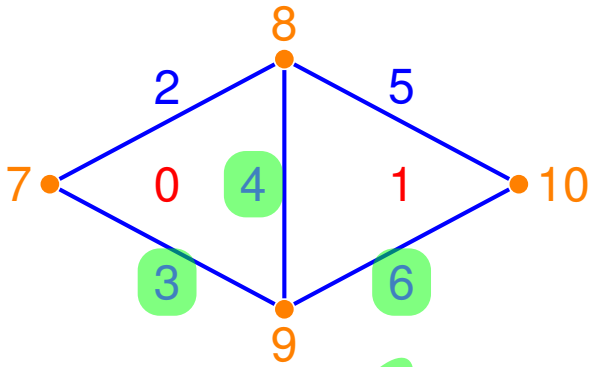


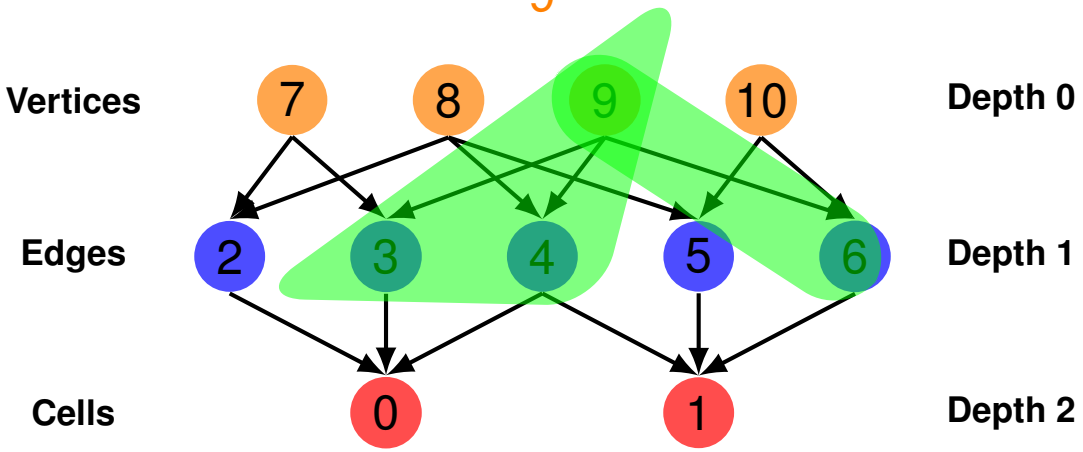


Basic Operations
Support

reverse arrows to get the dual operation,

support(9) = {3, 4, 6}

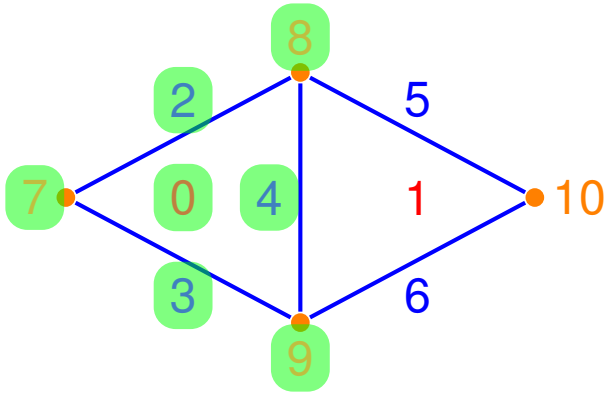


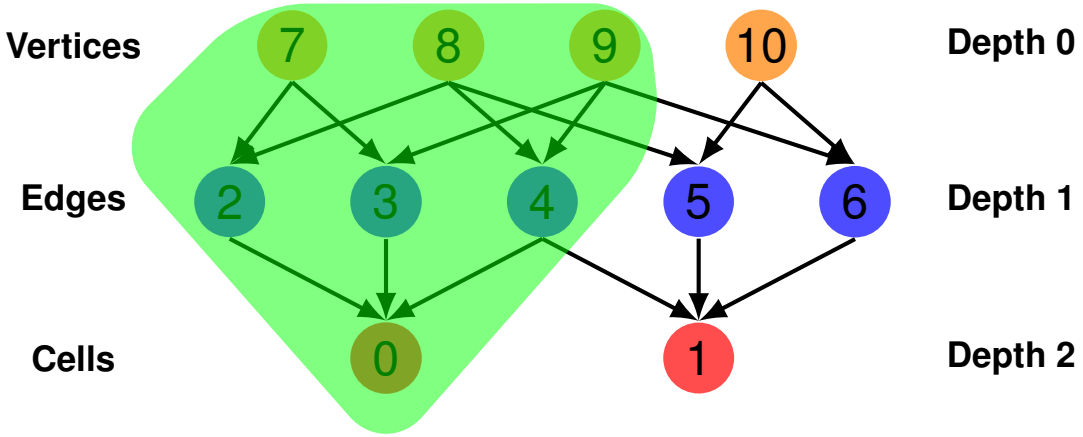


Basic Operations
Closure

add the transitive closure of the relation,

closure(0) = {0, 2, 3, 4, 7, 8, 9}



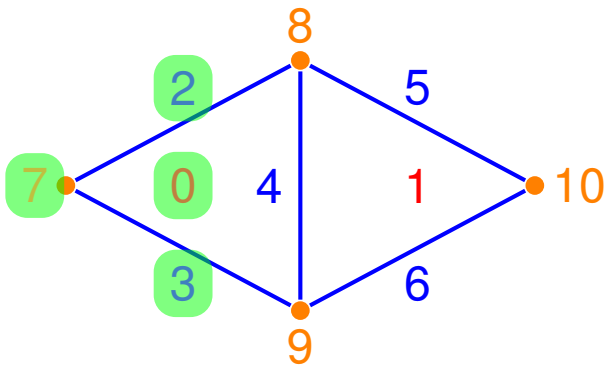


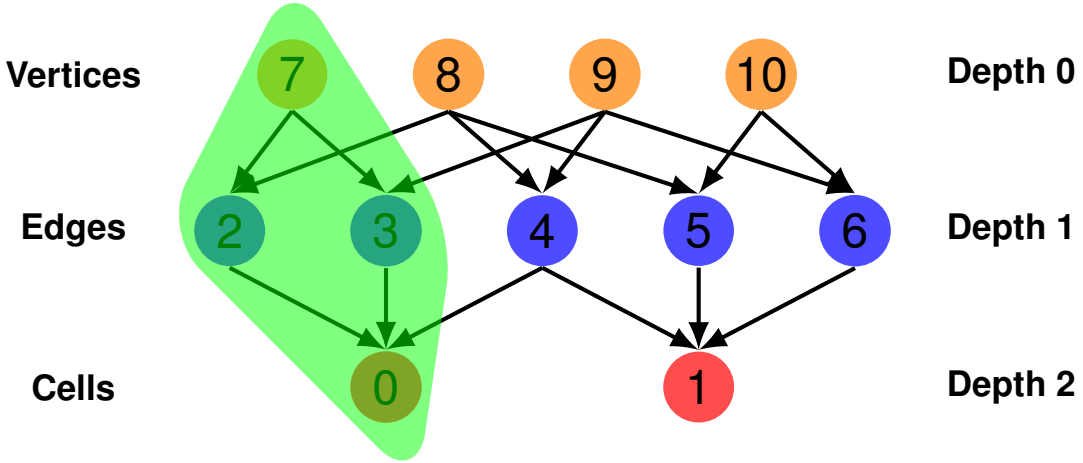
Basic Operations

Star

and the transitive closure of the dual,

star(7) = {7, 2, 3, 0}

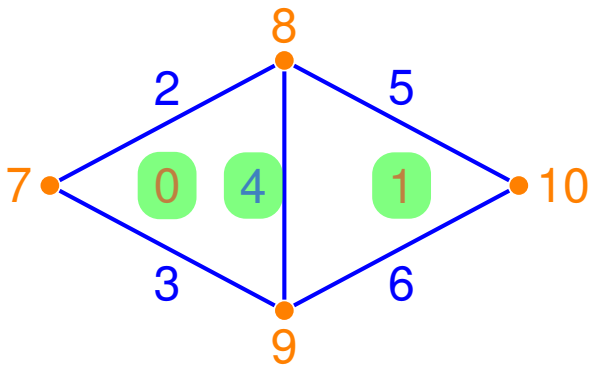


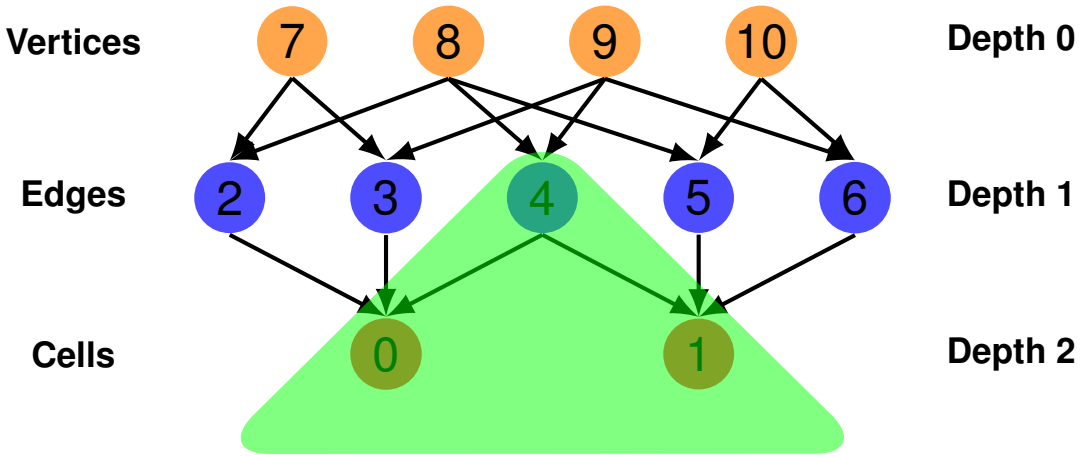


Basic Operations
Meet

and augment with lattice operations.

meet(0, 1) = {4}

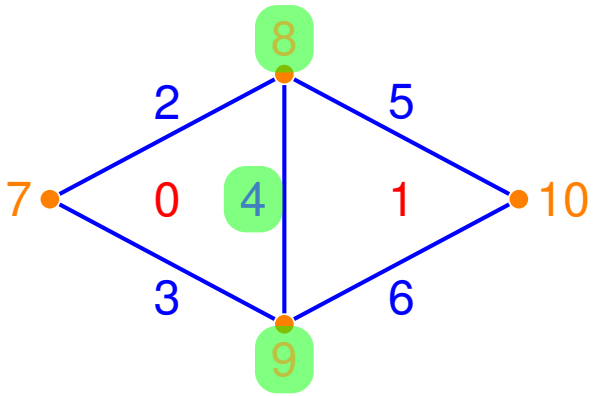


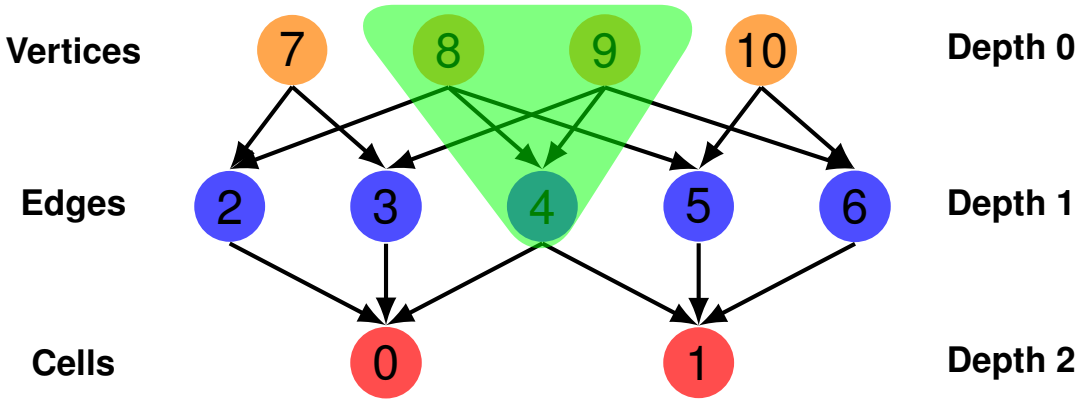


Basic Operations
Join

and augment with lattice operations.

join(8, 9) = {4}

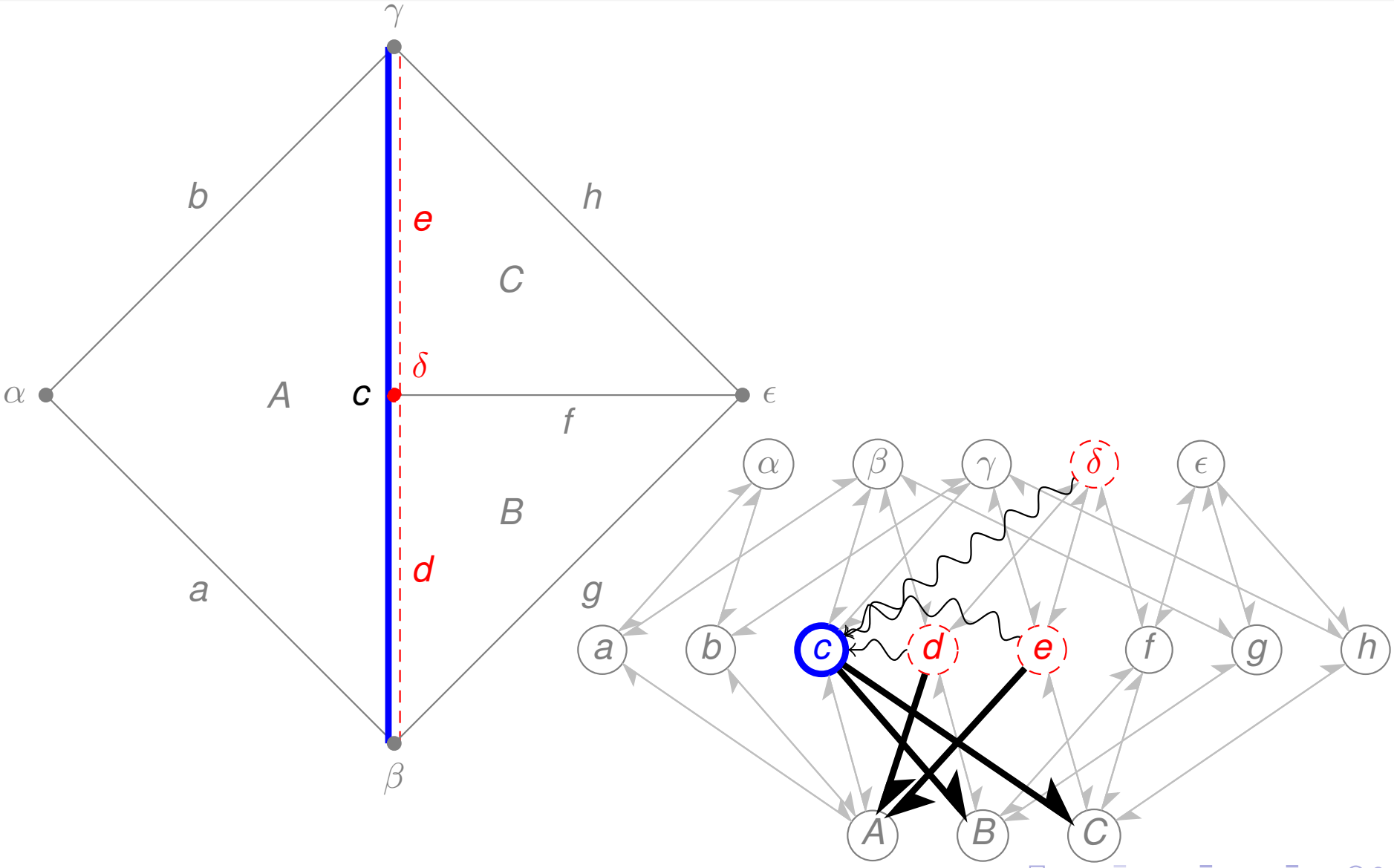




Outline

Nonconforming Doublet

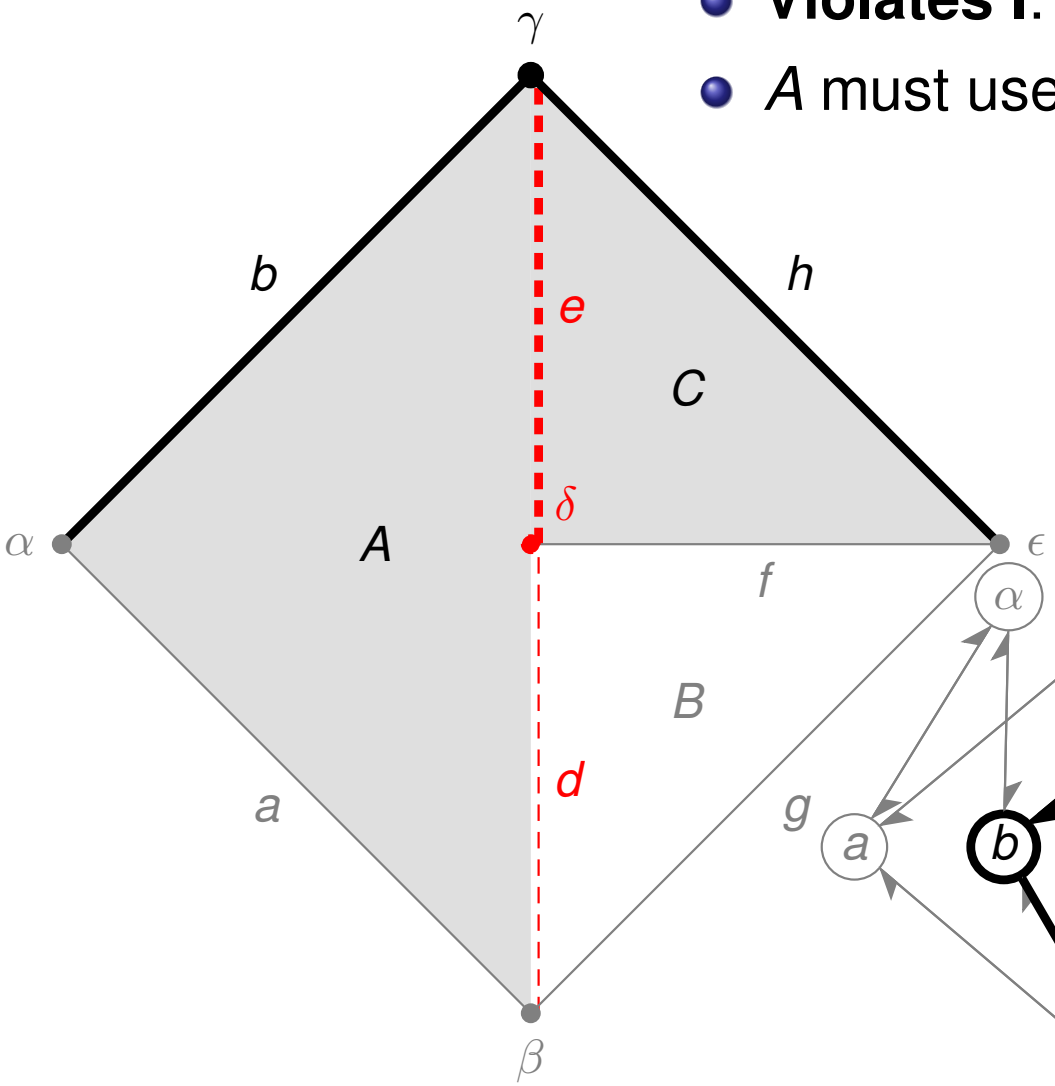
How to encode in Plex?

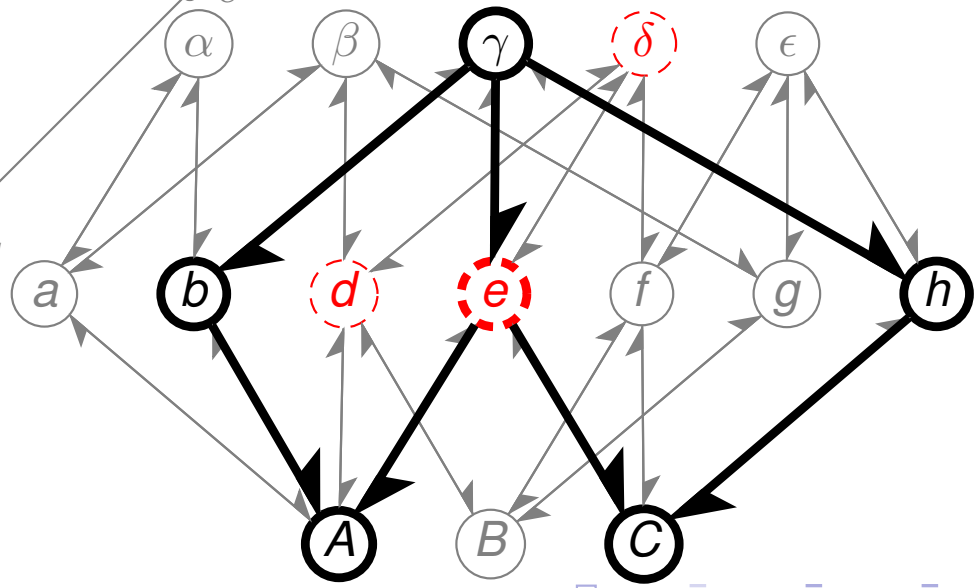


Nonconforming Doublet

Choice 1: Make A a degenerate quadrilateral

- **Violates I**: $B \in \mathrm{supp}(\gamma)$, but $B \notin \mathrm{star}(\gamma)$
- A must use a different element than B, C

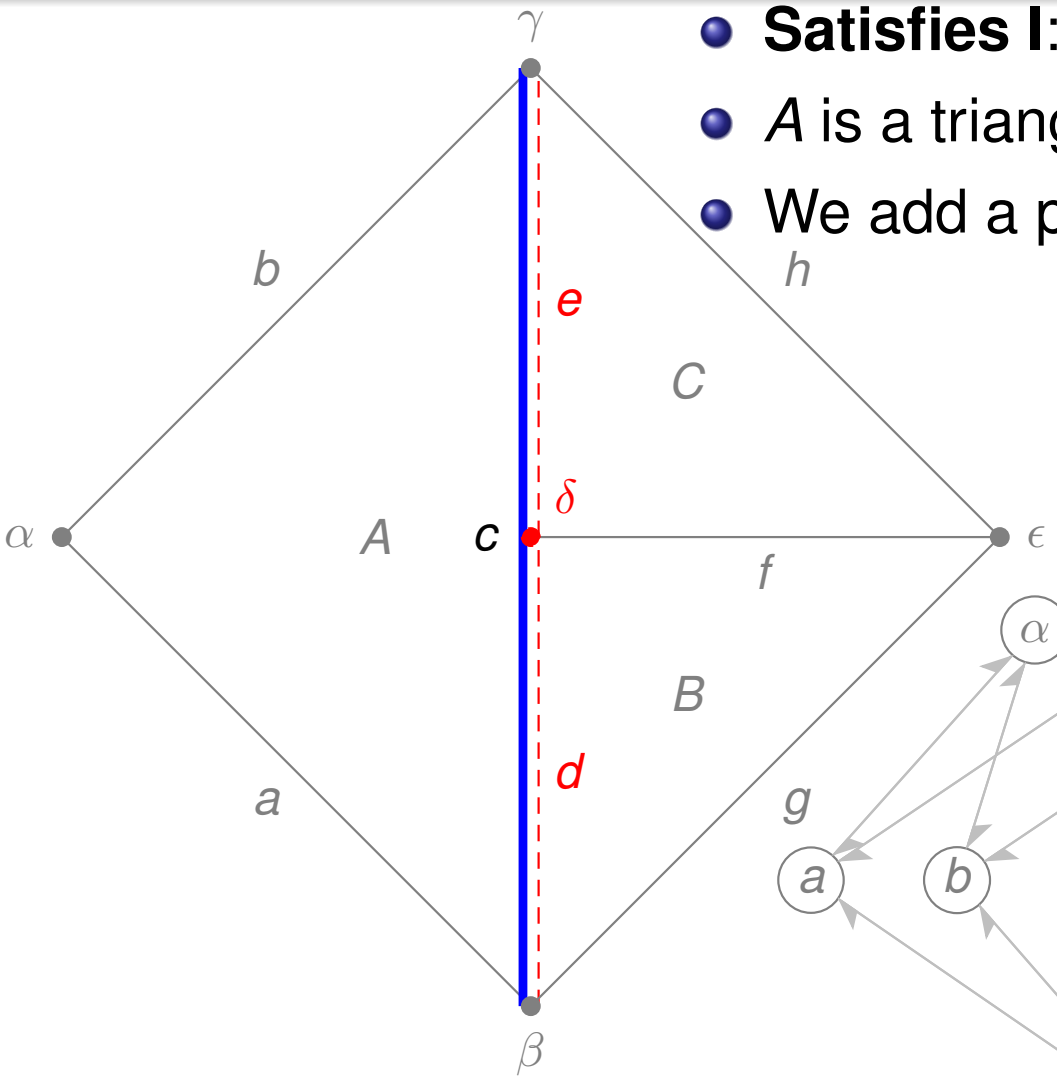


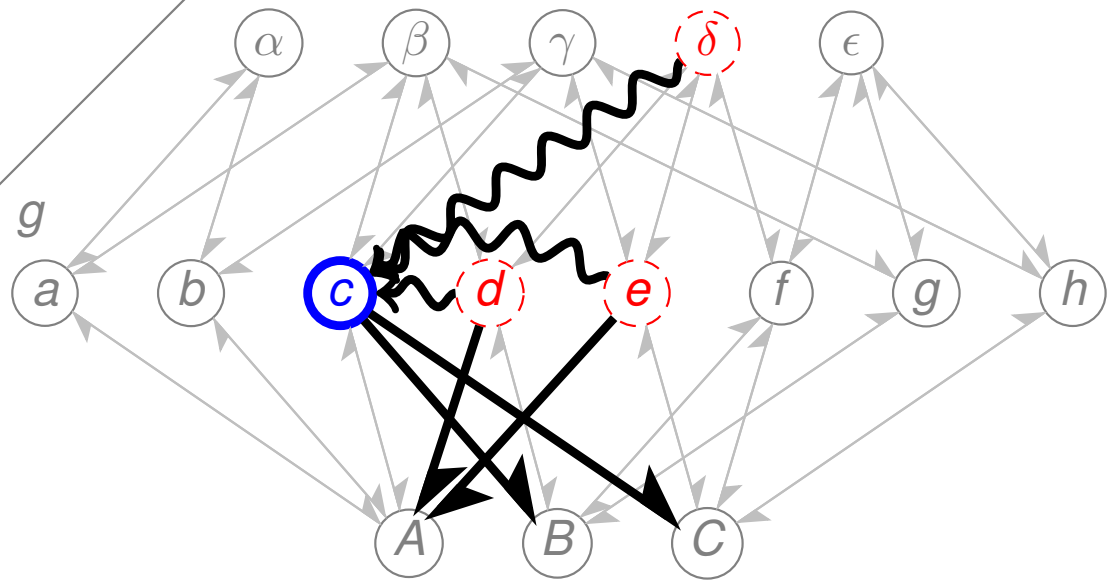


Nonconforming Doublet

Choice 2: Break cone-support duality

- **Satisfies I**: $B \in \mathrm{supp}(\gamma)$, and $B \in \mathrm{star}(\gamma)$
- A is a triangle element like B, C
- We add a parent-child relation





Outline

Dual Bases

In general, the union of all cell functionals

$$W^u = \bigcup_{i=1}^{N_T} \bigcup_{p \in S} Q_i^p$$

will contain linear dependencies. Instead, we use

$$W^c = \bigcup_{i=1}^{N_T} \bigcup_{\{p \in S : \mathrm{parent}(\varphi_i(p)) = \emptyset\}} Q_i^p.$$

and we must have a linear relation

$$W^u = I_c^u W^c$$

Creating I_c^u

If we have a child point p such that

- $p, q \in S$
- $\varphi_i(p) \subset \varphi_j(q)$
- $\varphi_j^{-1} \circ \varphi_i : p \to q$ is affine

then we can expand Q_i^p in terms of Q_j.

Creating I_c^u

For $\sigma_r \in Q^p$, by Axiom II,

$$
\begin{aligned}
(\varphi_{*,i}\sigma_r)(v) &= (\varphi_{*,i}\sigma_r)(\varphi_j^{-*}\varphi_j^* v) \\
&= (\varphi_{*,j}^{-1}\varphi_{*,i}\sigma_r)(\varphi_j^* v) \\
&= \sum_{\sigma_s \in Q} (\varphi_{*,j}^{-1}\varphi_{*,i}\sigma_r)(\psi_s)\sigma_s(\varphi_j^* v) \\
&= \sum_{\sigma_s \in Q_j} (\varphi_{*,j}^{-1}\varphi_{*,i}\sigma_r)(\psi_s)\sigma_s(v) \\
&= \sum_{\sigma_s \in \cup_{t \in \mathrm{clos}(\mathrm{parent}(p))} Q^t} (\varphi_{*,j}^{-1}\varphi_{*,i}\sigma_r)(\psi_s)\sigma_s(v).
\end{aligned}
$$

where we use Axiom I in the last line.

Creating I_c^u

Two Key Points:

- Sparsity of I_c^u
  We find *anchor points*, the points in clos of the transitive closure of $\mathrm{parent}(p)$ that are in W^c.
- Entries in I_c^u
  The matrix interpolates Q_i^p from its anchor point functionals. The entries have the form $(\varphi_{*,j}^{-1}\varphi_{*,i}\sigma_r)(\psi_s)$ for $\sigma_r \in Q$ and shape function $\psi_s \in P(K)$.

Creating I_c^u

Also, refinement usually follows a predictable pattern,

so we can evaluate the transfer functionals for the refined reference cell,

using a *reference tree* stored as a Plex,

and then map to an actual cell.

Creating I_c^u

```
/* Concatenate functionals of Q as pointsRef and weights                    */
EvaluateBasis(bspace,fSize,nPoints,sizes,pointsRef,weights,work,Amat);
/* Amat(i,j) evaluates basis i at dual basis functional j                   */
MatLUFactor(Amat,NULL,NULL,NULL);
/* loop over cells                                                          */
for (c = cStart; c < cEnd; c++) {
  DMPlexGetTreeParent(dm,c,&parent,NULL);
  if (parent == c) continue;
  /* Ref.  tree mappings are affine, corner (v0) and Jacobian (J)           */
  DMPlexComputeCellGeometryFEM(dm,c,NULL,v0,J,NULL,&detJ);
  DMPlexComputeCellGeometryFEM(dm,parent,NULL,v0parent,Jparent,invJparent,&detJpar);
  for (i = 0; i < nPoints; i++) {
    /* spdim is the spatial dimension                                       */
    /* push coordinates of functionals forward from child                   */
    CoordinatesRefToReal(spdim,spdim,v0,J,&pointsRef[i*spdim],vtmp);
    /* pull coordinates of functionals back to parent                       */
    CoordinatesRealToRef(spdim,spdim,v0parent,invJparent,vtmp,&pointsReal[i*spdim]);
  }
  EvaluateBasis(bspace,fSize,nPoints,sizes,pointsReal,weights,work,Bmat);
  /* Bmat(i,j) evaluates basis i at transfered functional j                 */
  MatMatSolve(Amat,Bmat,Xmat);
  /* ...  partition the columns of Xmat between the points in clos(c)       */
}
```

Creating I_c^u

If σ_r is associated with $p \in \mathrm{clos}(c)$,

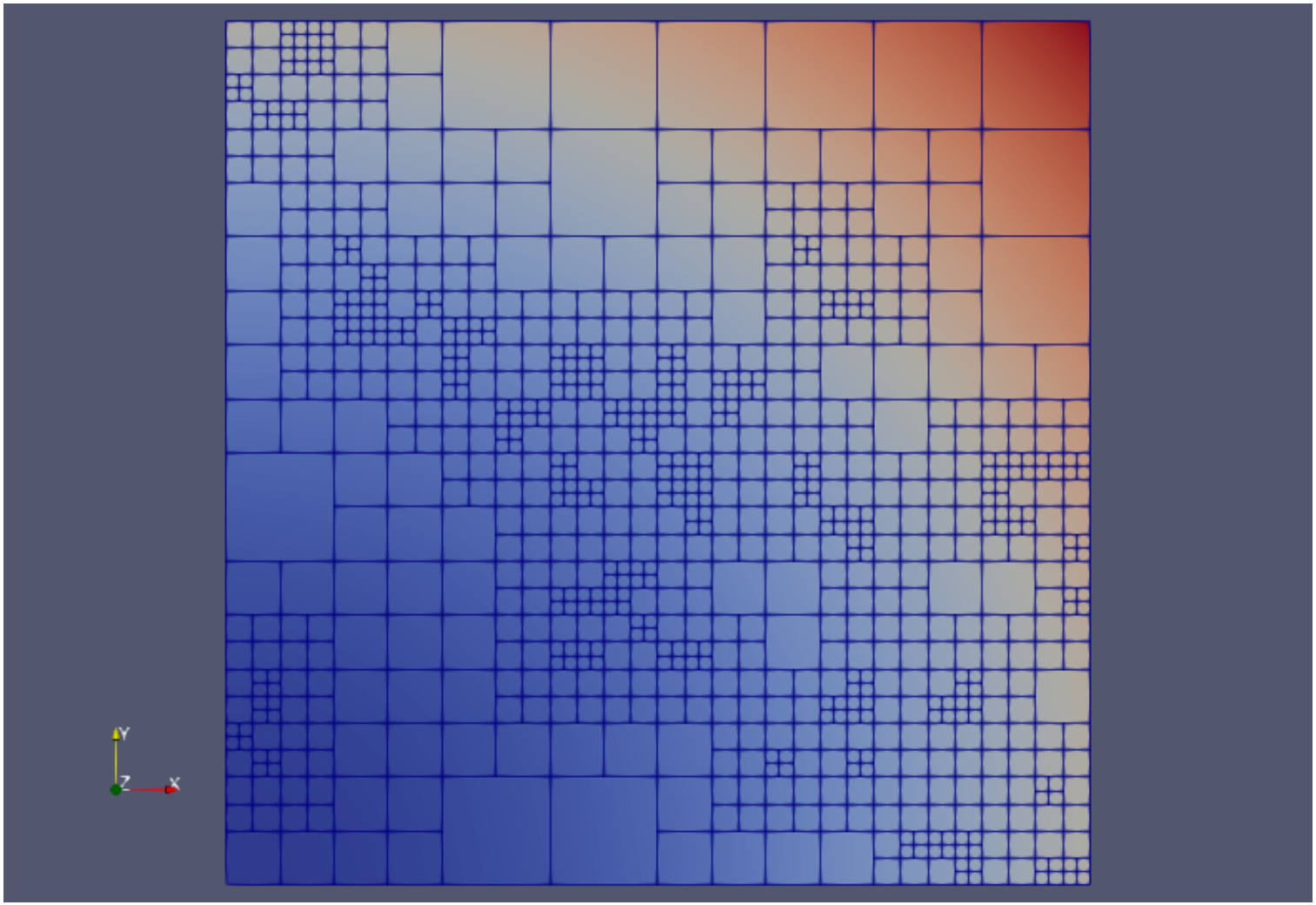
column r of X constrains σ_r to the dual basis of root cell $\mathrm{parent}(c)$,

X_{sr} is only nonzero if functional σ_s is associated to a point in $\mathrm{clos}(\mathrm{parent}(p))$.

Outline

Poisson with Finite Elements

A Poisson problem discretized with Q_2 elements



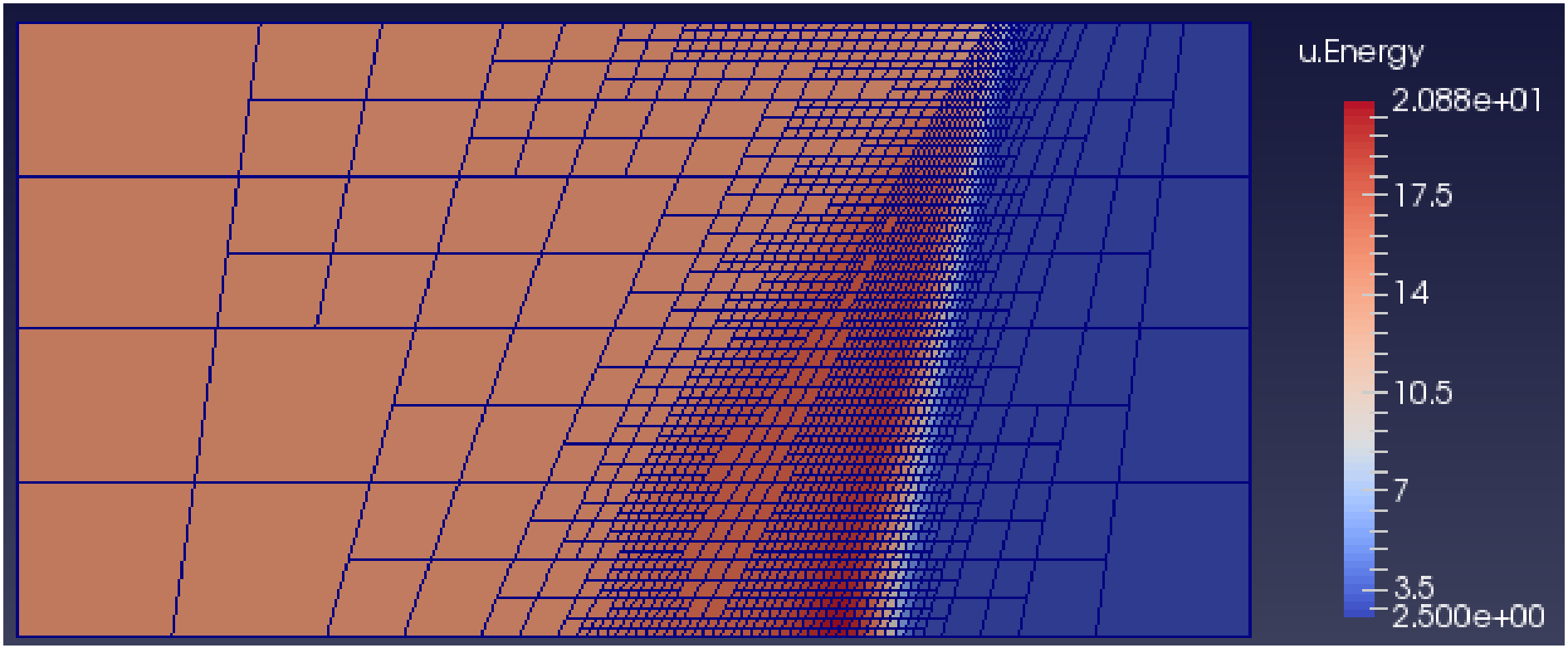
Poisson with Finite Elements

A Poisson problem discretized with Q_2 elements reproduced using SNES ex12:

```
./ex12 -run_type test -simplex 0 -interpolate 1
  -petscspace_order 2 -petscspace_poly_tensor
  -dm_plex_convert_type p4est -dm_forest_initial_refinement 2
     -dm_forest_minimum_refinement 0
     -dm_forest_maximum_refinement 6
     -dm_p4est_refine_pattern hash
  -dm_view vtk:amr.vtu:vtk_vtu
  -vec_view vtk:amr.vtu:vtk_vtu:append
```

Euler with Finite Volumes

A shock impinging on an oblique density contrast modeled using the Euler equation discretized with a TVD FV method



Euler with Finite Volumes

A shock impinging on an oblique density contrast modeled using the Euler equation discretized with a TVD FV method reproduced using TS ex11:

```
./ex11 -ufv_vtk_interval 1 -monitor density,energy -f -grid_size 2,1 -grid_bounds -1,1.,0.,1
    -bc_wall 1,2,3,4
 -dm_type p4est -dm_forest_partition_overlap 1 -dm_forest_maximum_refinement 6
    -dm_forest_minimum_refinement 2 -dm_forest_initial_refinement 2
 -ufv_use_amr -refine_vec_tagger_box 0.5,inf -coarsen_vec_tagger_box 0,1.e-2
    -refine_tag_view -coarsen_tag_view
 -physics euler -eu_type iv_shock -ufv_cfl 10 -eu_alpha 60. -grid_skew_60 -eu_gamma 1.4
    -eu_amach 2.02 -eu_rho2 3.
 -petscfv_type leastsquares -petsclimiter_type minmod -petscfv_compute_gradients 0
 -ts_final_time 1 -ts_ssp_type rks2 -ts_ssp_nstages 10
```

Advantages

Why is this good?

- Can do unstructured refinement as well
- Can do arbitrary refinements (not just 2:1)
- Can do arbitrary shapes (not just quads)
- Integrates seamlessly with solvers

Thank You!

http://www.caam.rice.edu/~mk51