ngsxfem: Geometrically unfitted discretizations with Netgen/NGSolve

(https://github.com/ngsxfem/ngsxfem)

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(with contributions from F. Heimann, J. Preuß, M. Hochsteger, ...)

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Geometry description via level sets

Level set function $\phi$

\[
\phi(x, t) = \begin{cases} 
  0, & x \in \Gamma(t), \\
  < 0, & x \in \Omega_1(t), \\
  > 0, & x \in \Omega_2(t).
\end{cases}
\]

Problems:
- PDEs on interior domain $\Omega_1$
- Interface problems involving $\Omega_1$, $\Omega_2$ and $\Gamma$
- PDEs on the interface $\Gamma$

Properties
- Description only \textit{implicit}
- Geometry evolution with \textbf{PDE for $\phi$}
- Meshes are \textit{unfitted}
Example problem 1: Stationary fictitious domain problem

Stationary geometrically unfitted domain ($\Gamma(t) = \Gamma$):

\[-\alpha \Delta u = f \quad \text{in} \quad \Omega = \{\phi < 0\},\]
\[-\alpha \nabla u \cdot n = g_N \quad \text{on} \quad \Gamma_N \subset \{\phi = 0\},\]
\[u = g_D \quad \text{on} \quad \Gamma_D \subset \{\phi = 0\}.\]

Features:

- "CutFEM": Finite element space $V_h^\Gamma = V_h|_\Omega$
- Imposition of Dirichlet values
  $\implies$ Lagrange multiplier / Nitsche techniques
- Weak formulations require integrals on $\int_\Omega \cdots dx$, $\int_{\Gamma} \cdots dx$:
  Numerical integration on cut elements
- Small cuts introduce stability and conditioning problems
  (stabilizations?!)
Example problem 2: Stationary interface problem

Stationary geometrically unfitted domain ($\Gamma(t) = \Gamma$):

\[-\alpha \Delta u = f \quad \text{in } \Omega_1 \cup \Omega_2,\]

\[-\alpha \nabla u \cdot n = 0 \quad \text{on } \Gamma,\]

\[\llbracket u \rrbracket = 0 \quad \text{on } \Gamma,\]

\[u = 0 \quad \text{on } \partial \Omega.\]

Features:

- Solution has kinks across $\Gamma$:
  - “CutFEM”: $V_{\Gamma}^h = V_h|_{\Omega_1} \oplus V_h|_{\Omega_2}$
  - or “XFEM”: $V_{\Gamma}^h = V_h \oplus V_h^x$

- Imposition of interface conditions
  \[\implies \text{Lagrange multiplier / Nitsche techniques}\]

- Numerical integration on \textit{cut elements}

- Small cuts (stability / conditioning)
Example problem 3: Stationary surface PDE problem (Laplace Beltrami)

Stationary geometrically unfitted domain ($\Gamma(t) = \Gamma$):

$$-\Delta_{\Gamma} u = f \quad \text{on} \ \Gamma.$$ 

Features:

- Solution defined only on $\Gamma$
  - "Trace/CutFEM": $V^{\Gamma}_h = V_h|_{\Gamma}$
- Numerical integration on cut elements
- Approximation of normal/tangential direction
- Ambiguity in normal directions
  $\Rightarrow$ (near) singular matrices (conditioning)
Example problem 4: Unsteady Poisson problem

Geometrically unfitted moving domain ($\Gamma(t) = \{\phi(x, t) = 0\}$):

\[
\begin{align*}
\partial_t u - \Delta u &= f \quad \text{in} \quad \Omega(t) = \{\phi(x, t) < 0\}, \\
- \alpha \nabla u \cdot n &= g_N \quad \text{on} \quad \Gamma_N(t) \subset \{\phi(x, t) = 0\}, \\
u &= g_D \quad \text{on} \quad \Gamma_D(t) \subset \{\phi(x, t) = 0\}, \\
u &= u_0 \quad \text{in} \quad \Omega(0) = \{\phi(x, 0) < 0\}.
\end{align*}
\]

Features:

- Time-dependent finite element spaces
- Space-Time:
  - Space-time finite element spaces
  - Numerical integration on space-time cut elements
- Characteristic FEM:
  - Characteristic back-tracking integrator
- + features of stationary unf. problems ...
Remarks on Examples 1-4

- Appear in two-phase flows
- Vector-valued versions relevant
  (Stokes interface, mean curvature calculation, ...)
- Background discretization can be conforming or nonconforming
Existing features

Related existing features in NGSolve:

- Background finite element spaces (scalar/vector, continuous/discontinuous)
- Convenient integral forms (VOL/BND/BBND)
- Handling of additional dofs: UNUSED_DOFs
- Easy set up of preconditioners
- Curved elements (isoparametric FE)
- Restriction of integration on some elements
- ...

\[
bfi = \text{SymbolicBFI}(u*v, \text{BND})
\]

\[
bfi.\text{SetDefinedOnElements}(...)\]
The new features of ngsxfem

New features in ngsxfem:

- **CutInfo** (level set cut topology):
  - Domain type per (VOL/BND) element:
    - **NEG**: completely in \( \{ \phi < 0 \} \)
    - **POS**: completely in \( \{ \phi > 0 \} \)
    - **IF**: intersected by \( \{ \phi = 0 \} \)
  - Cut ratio \( |T \cap \Omega_-|/|T| \) (detect small cuts)

- dof-handling for unfitted FE spaces, \( V_h = V_h|\Omega_- \)

- Extended FE spaces, \( V_h = V_h \oplus V_h^x \)

- Ghost penalty stabilization:
  - Marking of relevant facets (as BitArray)
  - Differential operator for \([\partial_n u]\) across facets

- **Numerical integration on cut elements**

Numerical integration on cut simplices

Tessellation

Approximation by piecewise linear level set function

\[ \Rightarrow \text{piecewise linear interface } \Gamma^{\text{lin}} \]

- explicit domain approx.
- robust
- 2nd order

\[
T_1 = T_a \cup T_b \cup T_c \\
T_2 = T_d
\]
Numerical integration on cut simplices

<table>
<thead>
<tr>
<th>Tessellation</th>
</tr>
</thead>
<tbody>
<tr>
<td>Approximation by piecewise linear level set function</td>
</tr>
<tr>
<td>$\Rightarrow$ piecewise linear interface $\Gamma^{\text{lin}}$</td>
</tr>
</tbody>
</table>

+ explicit domain approx.  + robust  − 2nd order

\[ T_1 = T_a \cup T_b \cup T_c \]

\[
\int_{\Omega^{\text{lin}}} f dx \quad \text{or} \quad \int_{\Omega^{\text{lin}}} uv dx \quad \text{in ngsxfem:}
\]

Integrate(levelset_domain={"levelset":lsetp1,"domain_type":NEG},cf=f)

SymbolicBFI(levelset_domain={"levelset":lsetp1,"domain_type":NEG},u*v)
Parametric mapping for higher order geometrical accuracy

Basic concept of isoparametric unfitted FEM

- Start from (multi-)linear level set $I_h \phi(h)$
Parametric mapping for higher order geometrical accuracy

- Higher order, implicit
- Low order, explicit
- Higher order, explicit

Basic concept of isoparametric unfitted FEM

- Start from (multi-)linear level set $l_h\phi(h)$
- Construct a mapping of the underlying mesh s.t. $l_h\phi \approx \phi \circ \Theta_h$
Parametric mapping for higher order geometrical accuracy

Basic concept of isoparametric unfitted FEM

- Start from (multi-)linear level set $I_h \phi(h)$
- Construct a mapping of the underlying mesh s.t. $I_h \phi \approx \phi \circ \Theta_h$

```python
lsetmeshadap = LevelSetMeshAdaptation(mesh, order=order)
defformation = lsetmeshadap.CalcDeformation(levelset) \rightarrow \Theta_h
mesh.SetDeformation(deformation)
```

Examples
Numerical integration in \texttt{ngsxfem}

Numerical integration on \textit{cut elements} with $\phi^{\text{lin}} + \text{mesh transformation } \Theta_h$

- Integration on linear level set domains on simplices:
  - Geometrical decomposition into simplices
- Integration by transformation to reference domain ($\Omega^{\text{lin}}$)
Numerical integration in ngsxfem

Numerical integration on cut elements with $\phi^{lin} + \text{mesh transformation } \Theta_h$

- Integration on linear level set domains on simplices:
  Geometrical decomposition into simplices
- Integration by transformation to reference domain ($\Omega^{lin}$)
  Transformation factors (det($D\Theta_h$), ...) are automatically considered due to NGSolves mesh deformation handling (ALETransformation)

Changes in quadrature ($\Omega^{lin}_i \rightarrow \Omega_{i,h} = \Theta_h(\Omega^{lin}_i)$)

Quadrature after mapping, $\text{dist}(\partial\Omega_i, \partial(\Omega_{i,h})) \leq O(h^{k+1})$, $\omega_i > 0$:

$$\int_{\Omega_i} f \, dx \approx \int_{\Omega_{i,h}} f \, dx = \int_{\Theta_h(\Omega^{lin}_i)} f \, dx \approx \sum_{T \in T_h} \sum_{i} \omega_i |\det(D\Theta_h(x_i))| f(\Theta_h(x_i))$$
Numerical integration in ngsxfem

Numerical integration on cut elements with $\phi^{\text{lin}} + \text{mesh transformation } \Theta_h$

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Consequences

- accuracy depends on $\Theta_h$, but cut topology of $\Omega_{i}^{\text{lin}}$ unchanged
- Guaranteed stability of quadrature: $\int_{\Omega_{i,h}} uv \, dx \simeq I_h(\Omega_{i,h}; uv)$,
  (positiveness of quadrature weights $\omega_i |\det(D\Theta_h(x_i))|$)
Mapping of quadrature points

quadrilaterals

triangles

deformed mesh $\Theta_h$ ($\mathcal{T}_h$)
deformation order: 1

undeformed mesh $\mathcal{T}_h$

integration order: 2

$\Theta_h \in (V_h^1)^2$

Mapping of quadrature points

quadrilaterals  triangles

defomed mesh $\Theta_h(T_h)$  undeformed mesh $T_h$
defomation order: 2  $\Theta_h \in (V^2_h)^2$
integration order: 4

Mapping of quadrature points

\begin{align*}
\text{quadrilaterals} & \quad \text{triangles} \\
\text{deformed mesh } \Theta_h(T_h) & \quad \text{undeformed mesh } T_h \\
deformation order: 3 & \quad \Theta_h \in (V_h^3)^2 \\
integration order: 6 &
\end{align*}
Mapping of quadrature points

(order = 4)

quadrilaterals  triangles

deformed mesh $\Theta_h(Th)$
undeformed mesh $Th$
deformation order: 4 $\Theta_h \in (V_h^4)^2$
integration order: 8

Jupyter demos!
Demands from unfitted FEM

- Handling cut information (cut elements ...)
- Numerical integration in cut elements
- Stabilization on parts of the mesh

Tools in ngsxfem

- CutInfo
- new FESpaces (XFESpace, SpaceTimeFESpace, ...)
- Levelset-domain integration for SymbolicBFI/LFI and Integrate
- **explicit** high order geometry approximation with trafo $\Theta_h$

Possibilities

- High order accurate unfitted FEM
- Simplex and quad meshes
- Fictitious domain / interface problems / surface PDEs
- Scalar and vector-valued problems
- Time dependent problem: ...
Outlook: Numerical integration in space-time in ngxsxfem

Space time integration

- Space-time FE for $\phi^{lin}$ (order $k_t$ in time, order 1 in space)
- Iterated integrals with space-time prism
  (in regions with same cut topology)
- Combine with space-time finite element for $\Theta_h : \Omega \times [t^{n-1}, t^n] \rightarrow \Omega$

```python
tfe = ScalarTimeFE(k_t)
fe = H1(mesh, order=1)
st_fes = SpaceTimeFESpace(fes,tfe)
lsetp1 = GridFunction(st_fes)
...
SymbolicBFI(levelset_domain={"levelset":lsetp1,..},u*v,time_order=4)
```

Thank you for your attention!

Questions / Comments?

https://www.github.com/ngsxfem/ngsxfem
https://www.github.com/ngsxfem/ngsxfem-jupyter