JSIAM annual meeting 4 Sep. 2019

An industrial application of a free boundary problem with contact angle and volume constraint

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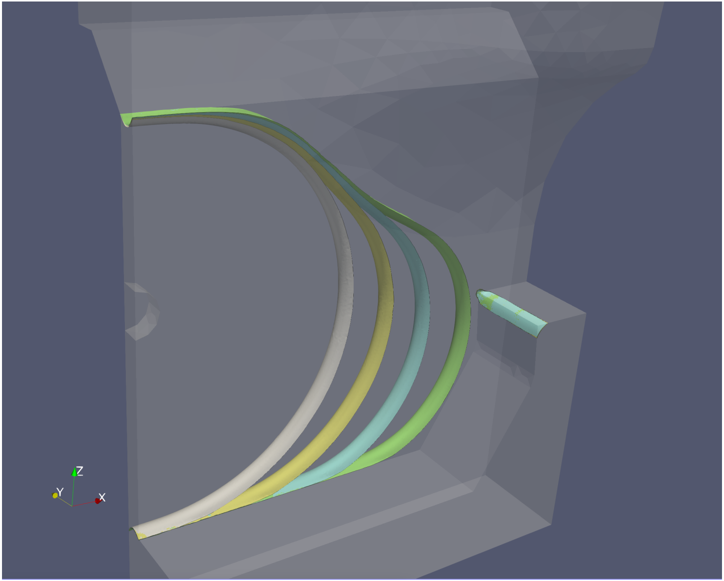
Joint work with DENSO to simulate a free boundary porblem

- aiming to replace COMSOL FEM analysis by FreeFEM
- more sophisticated numerical scheme than COMSOL
- pseudo time marching for gradient flow + stationary Newton iteration with 1.0$\sim$ 2.0 million unknowns on distributed parallel architecture
- volume conservation is treated within linear solver
- realistic computational geometry given by CAD software

`STEP` file by CAD software
`geo` file by Gmsh language
$\longrightarrow$
`FreeFEM`
`Gmsh` `HPDDM`
$\longrightarrow$ `ParaView`

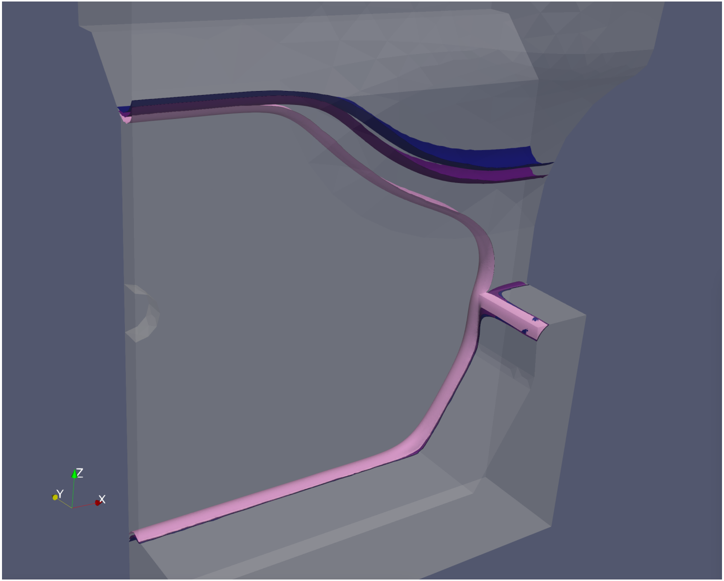
FreeFEM + Gmsh + HPPDM + $\alpha \gg$ COMSOL

computation of a model with $\theta = 30$



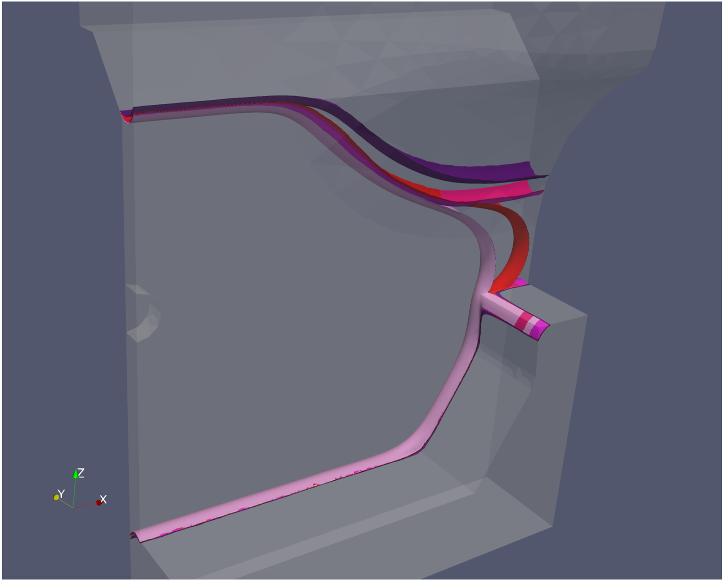
- liquid part is not yet reached to the other side but with leaking

computation of a model with $\theta = 30$



- liquid part has been reached to the other side with leaking

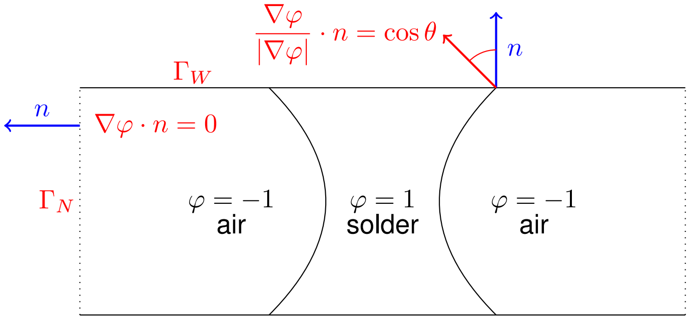
computation of a model with $\theta = 30$



- volume of the liquid part with filling has calculated by bisection

solder filling problem with contact angle

- indicator function : φ, solder : $\varphi = 1$, air : $\varphi = -1$.
- contact angle : $\dfrac{\nabla\varphi}{|\nabla\varphi|} \cdot n = \cos\theta$ on Γ_W
- volume conservation : $\displaystyle\int_\Omega \frac{\varphi + 1}{2} = V_0$
- free energy : $J(\varphi) := \dfrac{1}{2}\displaystyle\int_\Omega \kappa|\nabla\varphi|^2 + (\varphi+1)^2(\varphi-1)^2$ with $\kappa > 0$



variational setting : 1/3

set for solution embd. with boundary condi. and volume constraint

$$W(c, \cos\theta) := \left\{ \varphi \in H^{3/2}(\Omega)\,;\ \int_\Omega \varphi = c\,,\ \frac{\nabla\varphi}{|\nabla\varphi|}\cdot n = \cos\theta \ \text{ on } \Gamma_W\,, \right.$$
$$\left. \nabla\varphi \cdot n = 0 \ \text{ on } \Gamma_N \right\}\,.$$

$\partial\Omega = \Gamma_W \cup \Gamma_N$.

functional $\quad J : \Omega \to \mathbb{R}$ with $\kappa > 0$,

$$J(\varphi) := \frac{1}{2}\int_\Omega \kappa|\nabla\varphi|^2 + (\varphi+1)^2(\varphi-1)^2\,.$$

minimization of the energy

$$\varphi \in W(c, \cos\theta) \quad J(\varphi) \leq J(\psi) \quad \forall\psi \in W(c, \cos\theta).$$

variation of the energy

$\varphi \in W(c, \cos\theta)$, $\delta\varphi \in W(0, 0) \ \Rightarrow \ \varphi + \delta\varphi \in W(c, \cos\theta)$

$$J(\varphi+\delta\varphi) - J(\varphi) = \int_\Omega \kappa\nabla\varphi\cdot\nabla\delta\varphi + 2\varphi(\varphi^2-1)\delta\varphi + O(|\delta\varphi|^2).$$

suppose that an extremal attains the minimum of the energy

variational setting : 2/3

$\forall \delta\varphi \in W(0,0)$

$$\begin{aligned} 0 &= \int_\Omega \kappa \nabla\varphi \cdot \nabla\delta\varphi + 2\varphi(\varphi^2 - 1)\delta\varphi \\ &= \int_\Omega -\nabla \cdot \kappa\nabla\varphi\delta\varphi + \int_{\Gamma_W \cup \Gamma_N} \kappa\nabla\varphi \cdot n\delta\varphi + 2\int_\Omega \varphi(\varphi^2 - 1)\delta\varphi, \end{aligned}$$

by taking $\delta\varphi \in W(0,0) \cap H_0^1(\Omega)$

$$-\nabla \cdot \kappa\nabla\varphi + 2\varphi(\varphi^2 - 1) = 0 \quad \text{in } \Omega$$

definition of $W(c, \cos\theta)$ implies boundary conditions and volume constraint

$$\begin{aligned} \nabla\varphi \cdot n &= |\nabla\varphi| \cos\theta && \text{on } \Gamma_W\,, \\ \nabla\varphi \cdot n &= 0 && \text{on } \Gamma_N\,, \\ \int_\Omega \varphi &= c\,. \end{aligned}$$

variational setting : 3/3

affine space with volume constraint

$$V(c) := \left\{ \varphi \in H^1(\Omega)\,;\ \int_\Omega \varphi = c \right\}.$$

$$(F(\varphi), \psi) := \int_\Omega \kappa \nabla\varphi \cdot \nabla\psi + \int_\Omega 2\varphi(\varphi^2 - 1)\psi - \int_{\Gamma_W} \kappa |\nabla\varphi| \cos\theta\psi$$

$$\psi \in H^{1/2}_{00}(\Gamma_W), \nabla\varphi \in H^{-1/2}(\Gamma_W)^3$$

nonlinear stationary problem
find $\varphi \in V(c) \quad (F(\varphi), \psi) = 0 \quad \forall \psi \in V(0)$.

solved by Newton iteration

differential calculus
$\varphi \in V(c), \delta\varphi, \psi \in V(0)$

$$(F'(\varphi)\delta\varphi, \psi) = \int_\Omega \kappa \nabla\delta\varphi \cdot \nabla\psi + \int_\Omega (6\varphi^2 - 2)\delta\varphi\psi - \int_{\Gamma_W} \kappa \frac{\nabla\varphi \cdot \nabla\delta\varphi}{|\nabla\varphi|} \cos\theta\psi\,.$$

non-linear solver

Newton iteration
$\varphi^0 \in V(c)$: initial guess
loop $k = 0, 1, 2, \cdots$
find $\delta\varphi \in V(0)$

$$(F'(\varphi^k)\delta\varphi, \psi) = (F(\varphi^k), \psi) \quad \forall \psi \in V(0)$$

$$\varphi^{k+1} := \varphi^k - \delta\varphi$$

find $\delta\varphi \in V(0)$

$$\int_\Omega \kappa \nabla \delta\varphi \cdot \nabla \psi - 2 \int_\Omega \delta\varphi \psi + 6 \int_\Omega (\varphi^k)^2 \delta\varphi \psi - \int_{\Gamma_W} \kappa \frac{\nabla \varphi^k \cdot \nabla \delta\varphi}{|\nabla \varphi^k|} \cos\theta \psi$$
$$= \int_\Omega \kappa \nabla \varphi^k \cdot \nabla \psi + \int_\Omega 2\varphi^k((\varphi^k)^2 - 1)\psi - \int_{\Gamma_W} \kappa |\nabla \varphi^k| \cos\theta \psi$$
$$\forall \psi \in V(0)$$

- P2 finite element approximation to compute $\nabla \varphi^k$
- Newton iteration needs to start from an appropriate initial guess
  gradient flow solution with pseudo time marching
- $V(0) := \left\{ \varphi \in H^1(\Omega)\, ;\, \int_\Omega \varphi = 0 \right\}$: how to implement?

a way to find good initial guess for Newton iteration

gradient flow solution

an initial condition $\varphi(\tau)|_{\tau=0} = \varphi_0 \in V(c)$. $\dfrac{\partial \varphi}{\partial \tau} \to 0$ as $\tau \to +\infty$

$$\int_\Omega \frac{\partial \varphi}{\partial \tau} \psi = -(F(\varphi), \psi)$$

Crank-Nicolson scheme with $n+\frac{1}{2}$ - time step, $\varphi^{n+\frac{1}{2}} = \dfrac{\varphi^{n+1} + \varphi^n}{2}$,

$$\int_\Omega \frac{\varphi^{n+1} - \varphi^n}{\Delta \tau} \psi = -(F(\varphi^{n+\frac{1}{2}}), \psi)$$

Newton iteration at k-step with $\varphi_k^{n+\frac{1}{2}} = \dfrac{\varphi_k^{n+1} + \varphi^n}{2}$.

$$(F_{\mathsf{CN}}(\varphi_k^{n+1}, \varphi^n)\,, \psi) = \int_\Omega \frac{\varphi_k^{n+1} - \varphi^n}{\Delta \tau} \psi + (F(\varphi_k^{n+\frac{1}{2}})\,, \psi)$$

$$\begin{aligned}(F'_{\mathsf{CN}}(\varphi_k^{n+1}, \varphi^n)\delta\varphi\,, \psi) = {} & \int_\Omega \frac{\delta\varphi}{\Delta \tau} + \frac{1}{2}\int_\Omega \kappa \nabla \delta\varphi \cdot \nabla \psi - \int_\Omega \delta\varphi\psi \\ & + 3\int_\Omega (\varphi_k^{n+\frac{1}{2}})^2 \delta\varphi\psi - \frac{1}{2}\int_{\Gamma_W} \kappa \frac{\nabla \varphi_k^{n+\frac{1}{2}} \cdot \nabla \delta\varphi}{|\nabla \varphi_k^{n+\frac{1}{2}}|} \cos\theta\psi\end{aligned}$$

linear solver with constraint

Linear solver with Lagrange multiplier $\int_\Omega \varphi = c \;\Leftrightarrow\; \vec{m}^T\vec{\varphi} = c$
indefinite system (KKT type) : harder to solve even with coercive A

$$\begin{bmatrix} A & \vec{m} \\ \vec{m}^T & 0 \end{bmatrix} \begin{bmatrix} \vec{\varphi} \\ \lambda \end{bmatrix} = \begin{bmatrix} \vec{f} \\ c \end{bmatrix} .$$

block factorization with Schur complement $s = -\vec{m}^T A^{-1}\vec{m}$

$$\begin{bmatrix} A & 0 \\ \vec{m}^T & s \end{bmatrix} \begin{bmatrix} I & A^{-1}\vec{m} \\ 0 & 1 \end{bmatrix} \begin{bmatrix} \vec{\varphi} \\ \lambda \end{bmatrix} = \begin{bmatrix} \vec{f} \\ c \end{bmatrix} .$$

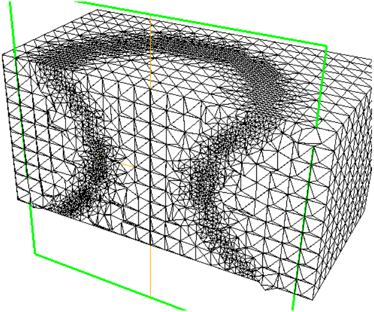
two linear solution with coercive (positive) matrix A

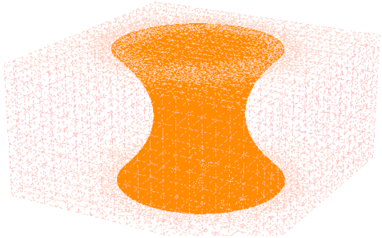
- solve $\vec{w}$: $A\vec{w} = \vec{m}$
- $s = -\vec{m}^T\vec{w}$
- solve $\vec{\varphi}$: $A\vec{\varphi} = \vec{f}$
- solve λ : $s\lambda = c - \vec{m}^T\vec{\varphi}$
- $\vec{\varphi} = \vec{\varphi} - \lambda\vec{w}$

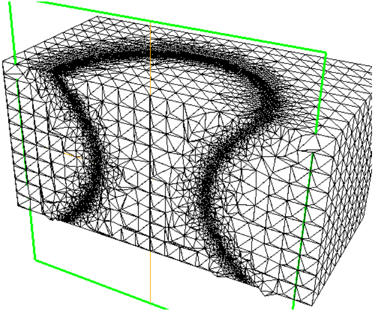
question : A is coercive, $(A + A^T)/2 > 0$?
... seems to be ok with good initial guess of Newton iteration

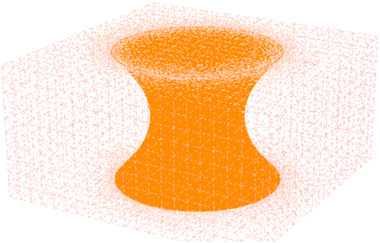
An algorithm to find extremal with mesh refinement : 2/2

mesh refinement by `mmg3d`









computational efficiency with FreeFEM

performance of an academic problem

level	# unknowns	refinement parameter
0	35,301	uniform mesh $20 \times 20 \times 10$, $h = 0.1$
1	461,573	$\lvert\varphi\rvert < 0.6 : h/4,\ \lvert\varphi\rvert < 0.9 : h/2$
2	1,693,049	$\lvert\varphi\rvert < 0.3 : h/8,\ \lvert\varphi\rvert < 0.6 : h/4,\ \lvert\varphi\rvert < 0.9 : h/2$
3	1,781,054	$\lvert\varphi\rvert < 0.3 : h/8,\ \lvert\varphi\rvert < 0.6 : h/4,\ \lvert\varphi\rvert < 0.9 : h/2$
4	1,792,096	$\lvert\varphi\rvert < 0.3 : h/8,\ \lvert\varphi\rvert < 0.6 : h/4,\ \lvert\varphi\rvert < 0.9 : h/2$

level	# unknowns	# Newton	PARDISO	additive Schwarz	AMG
0	35,301	7	12.048	10.937	8.198
1	461,573	8	320.845	271.790	347.003
2	1,693,049	5	1,107.044	919.195	703.402
3	1,781,054	4	996.045	802.735	602.678
4	1,792,096	4	1,024.829	807.679	615.471
total (sec.)			3,510.67	2,919.68	2,352.85

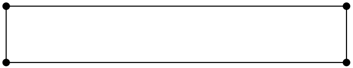
Intel Core i7-6770HQ CPU @ 2.60GHz 4 cores

performance of acutual geometry

package	hpddm	hypre
preconditioner	additive Schwarz	AMG
# iteration	12	116
time (sec.)	4.848	17.199

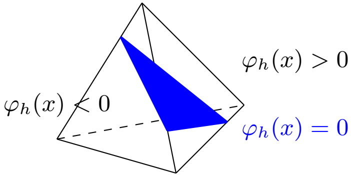
Computation of Euler characteristic : 1/2

stripe shape of the interface between solid and liquid part



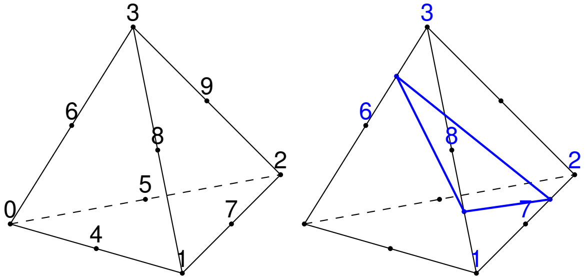
$$\text{Vertex} = 4$$
$$\text{Edge} = 4$$
$$\text{Face} = 1$$
$$V - E + F = 4 - 4 + 1 = 1$$

indicator function $\varphi_h(x)$ by P2



element-wise detection of zero iso-surface approximated by P1

Computation of Euler characteristic : 2/2



edges of
$\varphi(x) = 0$
(3,6) — (1,8)
(1,8) — (2,7)
(2,7) — (3,6)

- perturbe $\varphi(P_k) = 0\ (0 \leq k < 10)$ with $\varepsilon > 0$ to avoid zero surface passing on P2 nodes
- edge of triagle of zero surface $\varphi = 0$ is shared with other elements
- presence of edge of the surface triangle is registerd as an entry of CSR sparse matrix

implementation	time (sec.)	core
FreeFEM script	248.85	1
FreeFEM script	196.23	6 : parallel only over elements
C++ dynamic loading	2.15	1

in C++ implementation CSR matrix is managed by STL list

C++ coding to extend FreEFEM with dynamic loading : 1/2

function to compute Euler characteristic and number of liquid/sold domain

`checkconnectivity(mesh3 Th3, real[int] &gg,int[int] &ivars)`

	FreeFEM script	C++ function
input	`mesh3 Th3`	`atype<Mesh3 *>`
	`real[int] &gg`	`atype<KN<double> *>`
output	`int[int] &ivars`	`atype<KN<long> *>`

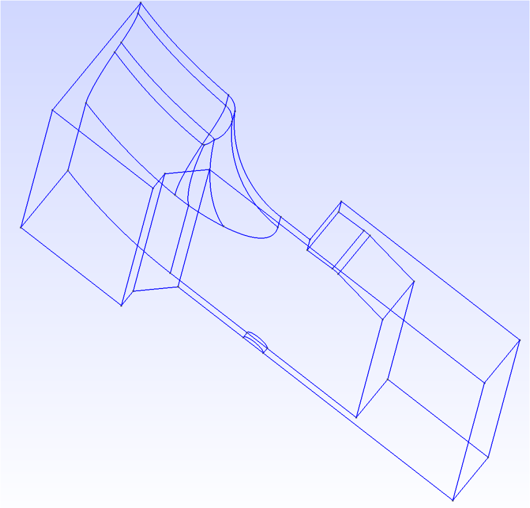
FreeFEM script : cf. 6.14 Finite elemens connectivity

```
mesh3 Th;
fespace Vh(Th, P2);
for (int k = 0; k < Vh.nt; k++) {
  for (int j = 4; j < 10; j++) { // running middle nodes of P2
    int ii = Vh(k, j);
```

C++ implementation : cf. `femlib/FESpace.hpp`

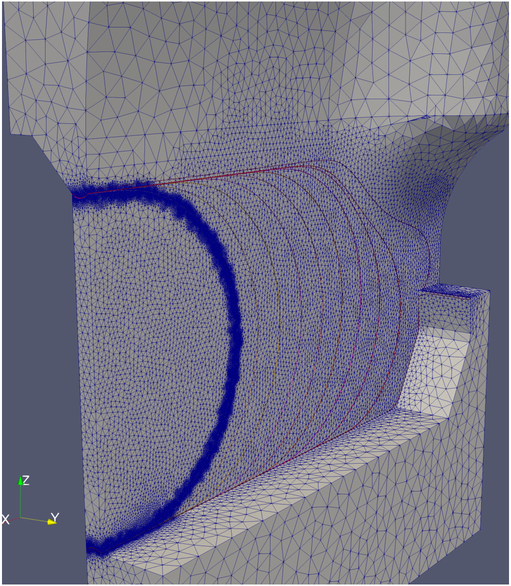
```
Mesh3 *pTh;
FESpace3 *pVh = new FESpace3(*pTh, DataFE<Mesh3>::P2);
FESpace3 &Vh = *pVh;
for (int k = 0; k < Vh.NbOfElements; k++) {
  for (int j = 4; j < 10; j++) { // running middle nodes of P2
    int ii = Vh(k, j);
```

STEP file that is directly read by Gmsh



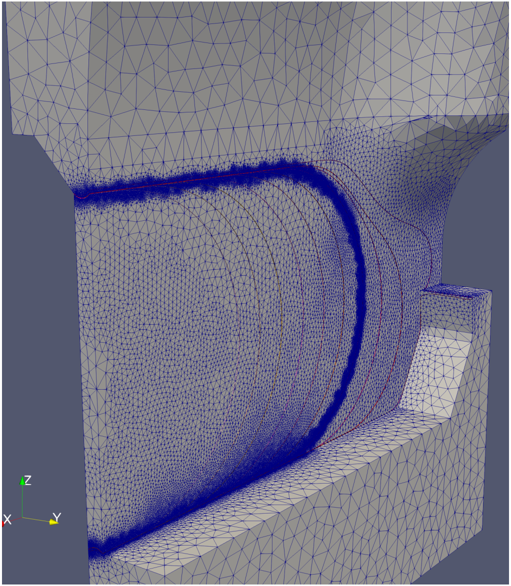
- using OpenCASCADE geometry engine
- setting of boundary conditions with geo file which includes STEP file

numerical result by dynamic refinement strategy : 1/5



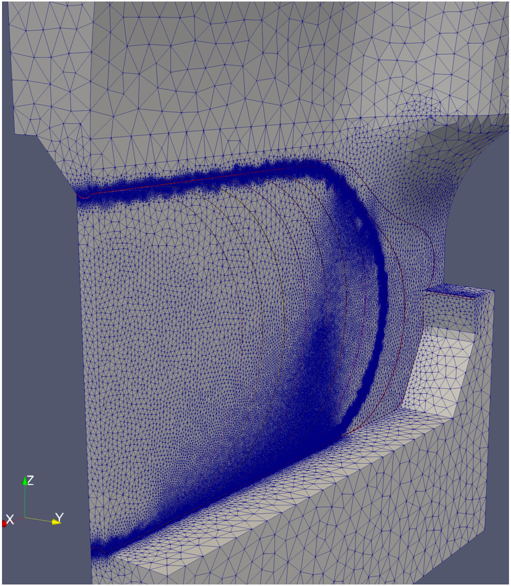
$\theta = 45$ degree, volume = 0.955323

numerical result by dynamic mesh refinement strategy : 2/5



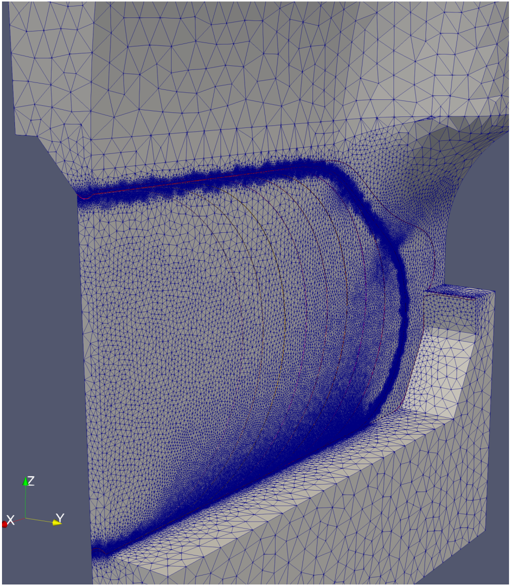
$\theta = 45$ degree, volume = 2.66561

numerical result by dynamic mesh refinement strategy : 3/5



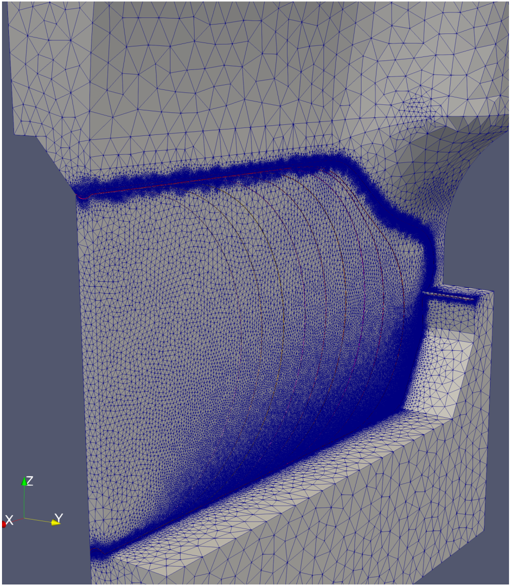
$\theta = 45$ degree, volume = 2.96374

numerical result by dynamic mesh refinement strategy : 4/5



$\theta = 45$ degree, volume = 3.26019

numerical result by dynamicmesh refinement strategy : 5/5



$\theta = 45$ degree, volume = 3.79139

conclusion

- Contact angle condition and volume constraint are imposed on the set to find a solution.
- Nonlinear boundary value problem is solved by Newton iteration with an initial guess that is obtained by pseudo time marching of gradient flow problem.
- Newton iteration combined with mesh refinement can find nonlinear solution efficiently.
- Volume constraint is treated as linear constraint for the linear system. Resulting system is a KKT type consisting of indefinite matrix and it is solved by two stages using Schur complement matrix.
- C++ implementation to compute Euler characteristics drastically shortens the computational time by FreeFEM script

FreeFEM on cloud

- `http://www.rescale.com` in conjunction with DENSO

FreeFEM + Gmsh + HPPDM + $\alpha \gg$ COMSOL
$\alpha \in \{$ nonlinear solver, time integration, optimization algorithm $\}$

Thanks to F. Hecht, P. Jolivet, S. Garnotel, F. Lahaye, and H. Ogawa