Phase field modelling

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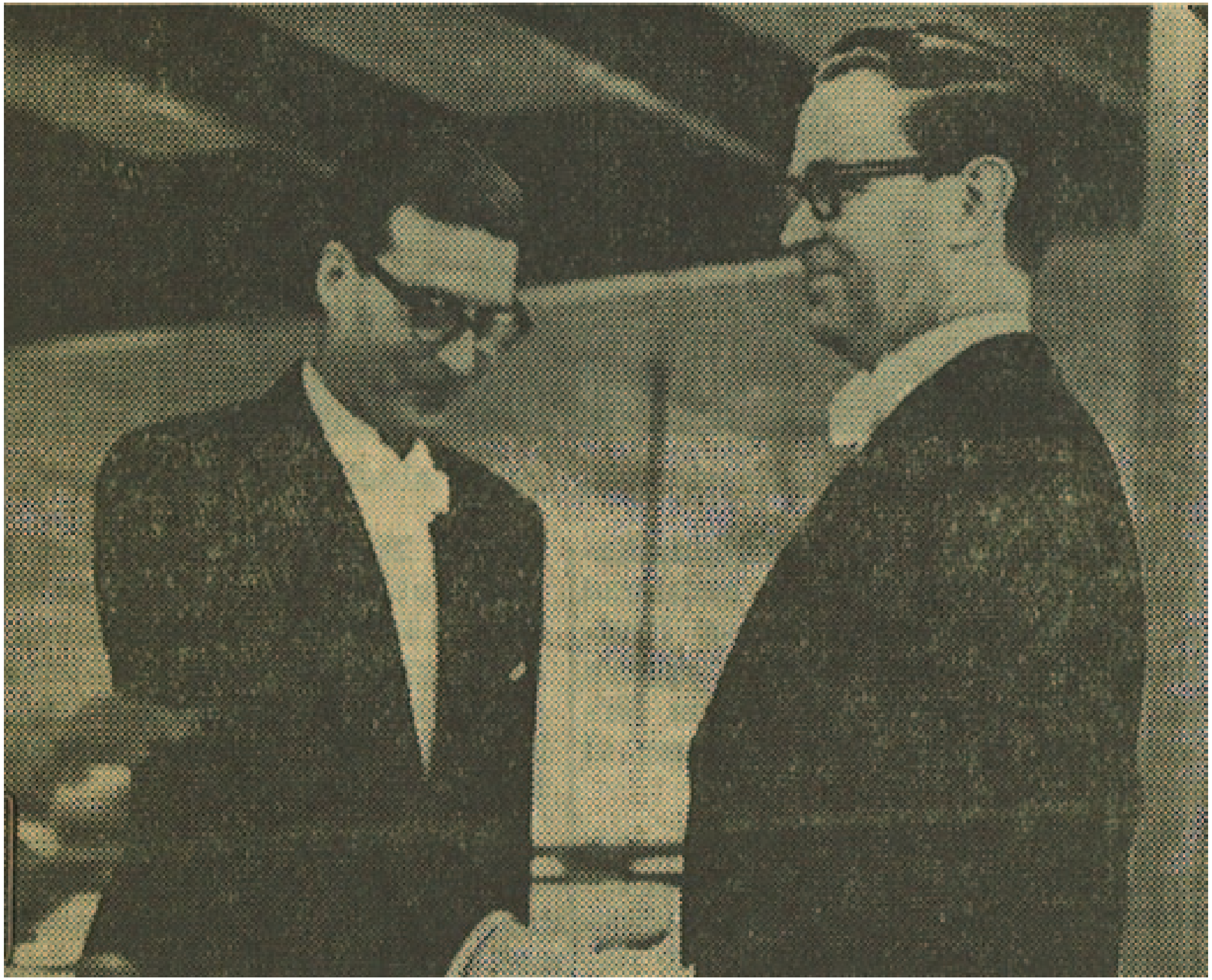

LUND UNIVERSITY

IMS/ISSEC SYMPOSIUM, Dublin 2013

Stress Corrosion Using Phase Field Modelling

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U. Hejman, E. Hansen

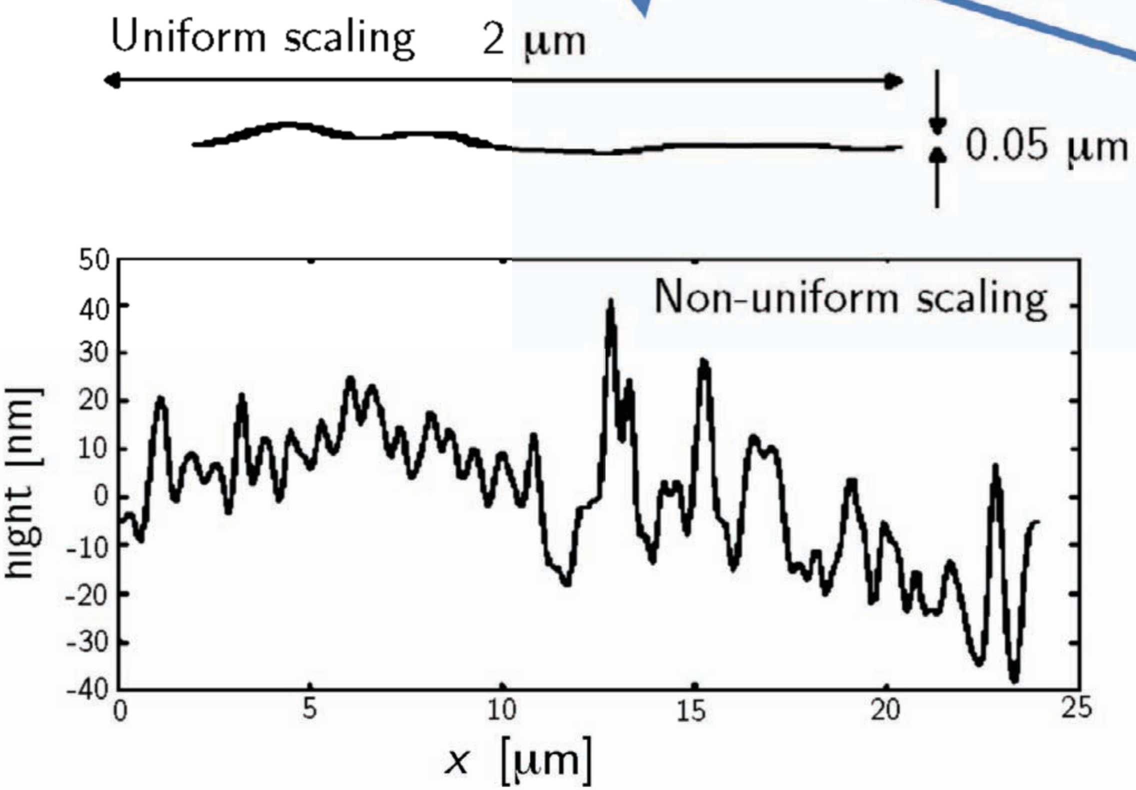
Corroding environment leads to:

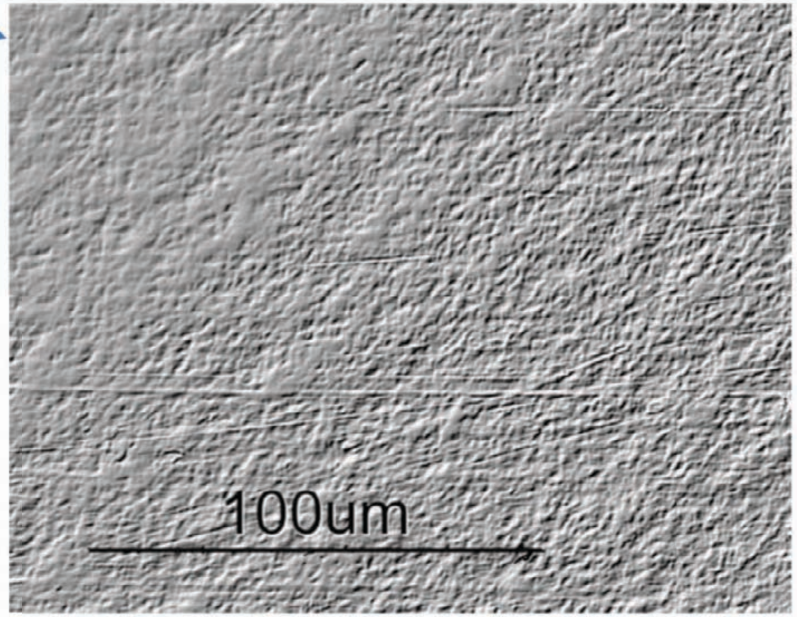
1. Continuous loss of mass
2. Pitting

... and with mechanical stress present

3. Surface roughening

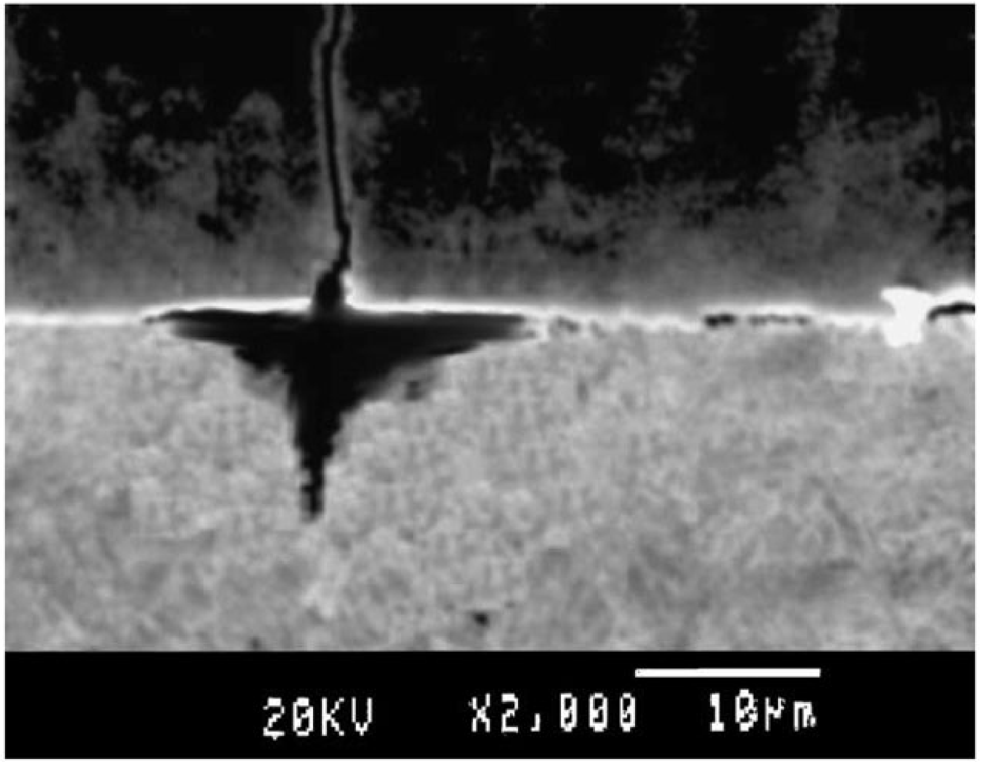
(from Kim *et al.* 2000)





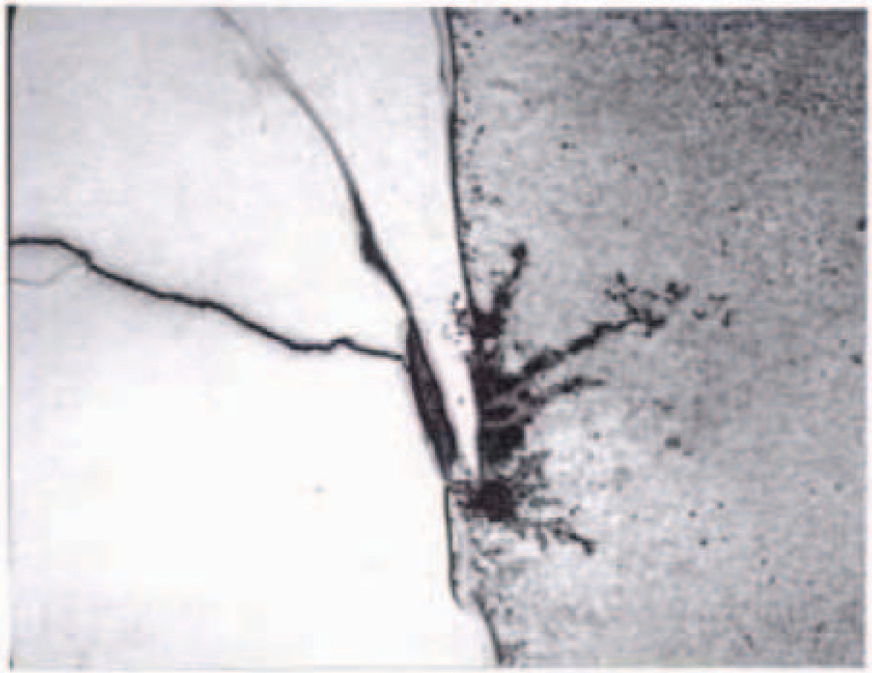
4. Evolving pits
5. Formation of cracks
6. Crack growth
7. Crack branching

Growing crack in a polycarbonate exposed to acetone (Hejman 2011)

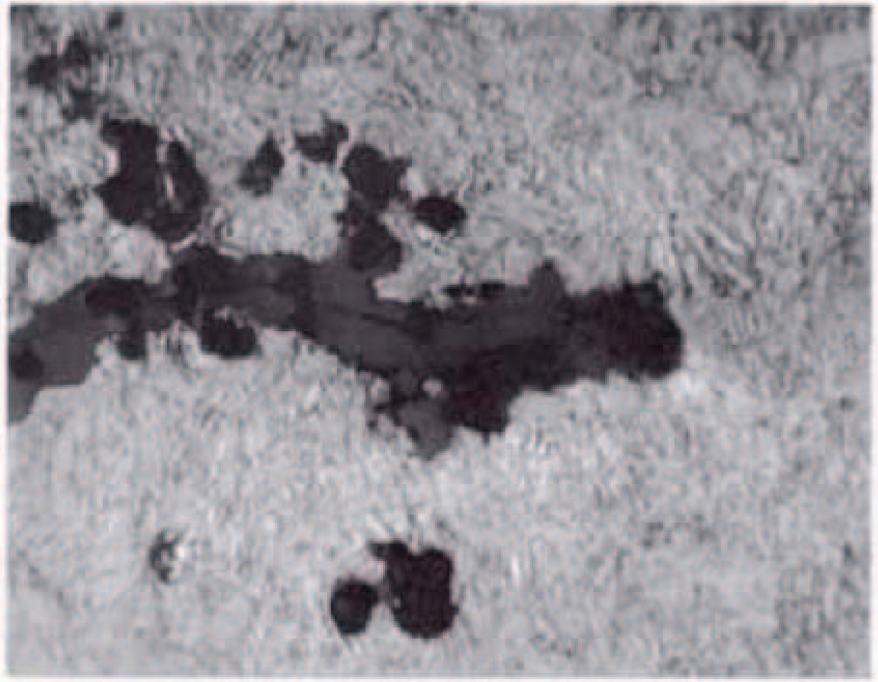


Cr/zone six charge related of land and groove substrate erosion through a micro-crack at the 12:00 bore origin. (Sopok *et al.* 2005)

Corrosion Crack crossing a bi-material interface



Corrosion crack penetrating a bimaterial interface between austenitic and pressure vessel steel of type SA533C11.



The tip of one of the crack branches. Crack length 7 mm, notch width 10 μm. *Reproduced with permission from Vattenfall AB.*

Biocorrosion

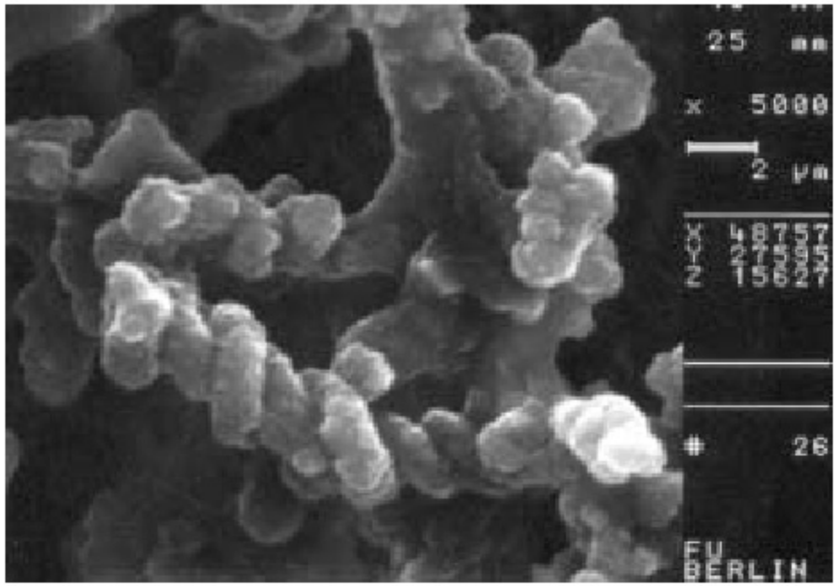
Known to cause SC

Anaerobic Bacteria: *Desulfovibrio, -maculum, -monas , Gallionella*

Aerobic Bacteria: *Thiobacillus*

Fungi, Algae, Protozoans

Corrosion in stainless cased by Gallionella Bacillus. ASTM.



SEM image Gallionella ferruginea in a biofilm network. Halbach,*et al*, 2001.

Energies contributing to the body evolution

Contributions to the free energy (Ginzburg & Landau, 1950)

$$\mathcal{F} = \mathcal{F}_{el} + \mathcal{F}_{ch} + \mathcal{F}_{gr}$$

Volume totals:

Elastic energy $\quad \mathcal{F}_{el} = \int \frac{G(\psi)}{2}(\nabla w)^2 dV$

Chemical energy $\quad \mathcal{F}_{ch} = \int U(\psi)\, dV$

Gradient energy $\quad \mathcal{F}_{gr} = \int \frac{g_b}{2}(\nabla \psi)^2 dV$

Antiplane deformation $=>$ Two free variables

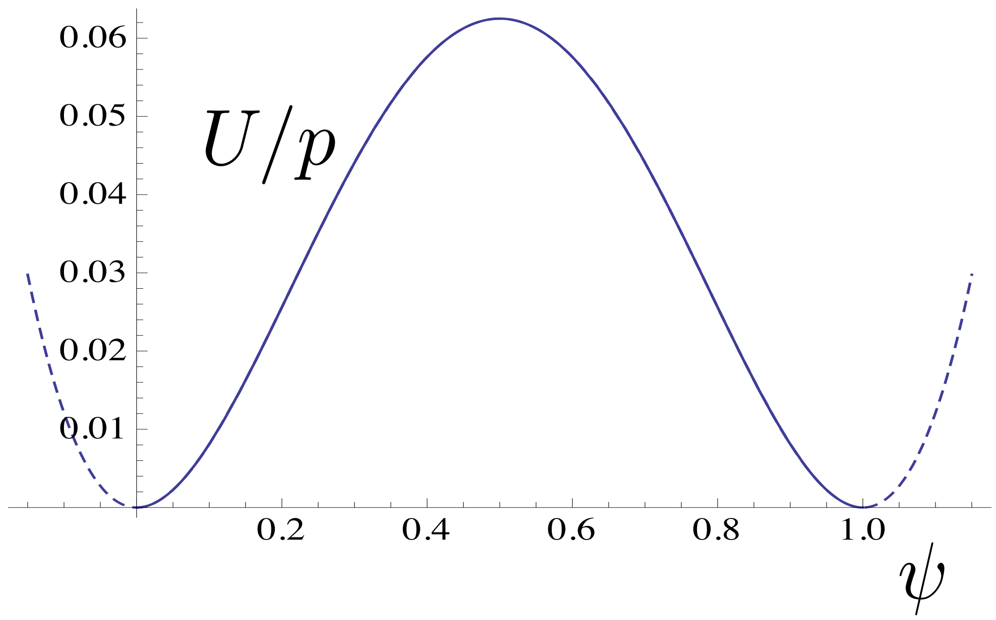
Displacements w and phase (density) ψ

$$\frac{\partial \psi}{\partial t} = -L_\psi \frac{\delta \mathcal{F}}{\delta \psi} \quad , \qquad \frac{\partial w}{\partial t} = -L_w \frac{\delta \mathcal{F}}{\delta w}$$

Ginzburg, Landau (50)

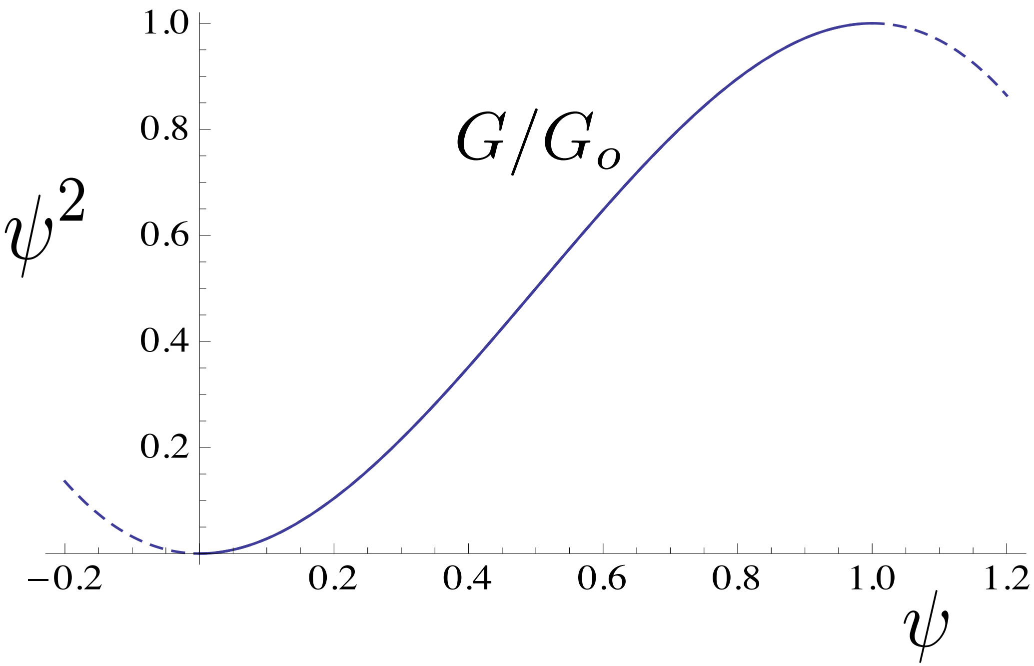
Double-well chemical potential

$$U(\psi) = p\,\psi^2(1-\psi)^2$$



Shear modulus

$$G(\psi) = G_o(\psi)(-2\psi + 3)\psi^2$$



Gradient Energy

$$\frac{g_b}{2}(\nabla\psi)^2$$

Variation with respect to ψ: $g_b \triangle \psi$

Fickean diffusion

$$\frac{\partial \psi}{\partial t} = L_\psi g_b \triangle \psi]$$

Evolution of the phase

$$\frac{\partial \psi}{\partial t} = -L_\psi [\frac{1}{2} G'(\psi)(\nabla w)^2 + p\psi(\psi^2 - 1) - g_b \triangle \psi]$$

Evolution of the displacements

$$\frac{\partial w}{\partial t} = L_w \nabla \cdot [G(\psi) \nabla w]$$

At equilibrium: $\nabla \cdot [G(\psi) \nabla w] = 0$

Surface Morphology:
Surface Wave Spectrum

Crack Initiation:
Pit, Cusp and Crack

Crack Growth:
Crack Growth, Blunting and Branching

Evolving Surface Morphology

Asaro-Tiller (1972), Grinfeld (1986, 1993), Srolovitz (1989), Freund (1995), Kim (2000)

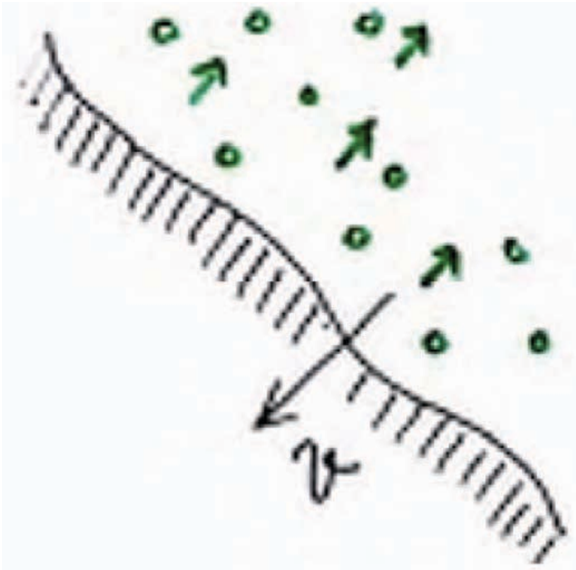
Gibb's free energy

$$\Phi = U_c + U_e$$

where

U_c is the free chemical energy and
U_e is the free elastic energy

Evaporation-condensation



$$\frac{\partial h}{\partial t} = -L_1 \Phi$$

Surface diffusion

$$\frac{\partial h}{\partial t} = L_2 \frac{\partial^2 \Phi}{\partial x^2}$$

Nearly Plane Surface:

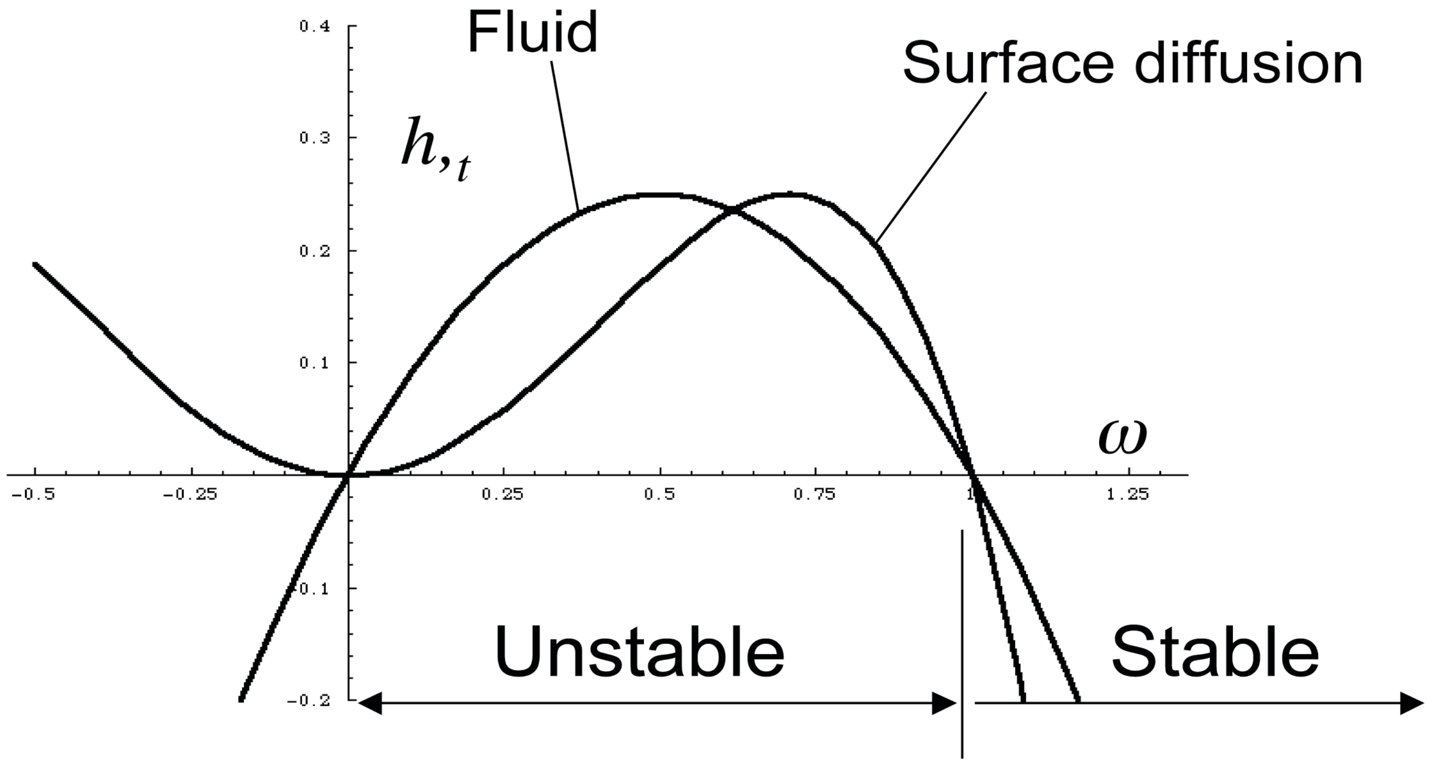
Fouriertransform, put $h = A \sin\omega x \qquad |A| << x$

<u>Surface Diffusion</u>

$$h_{,t} = D[(\mu/2)\varepsilon_o\,\omega^3 - \gamma\omega^4]h$$

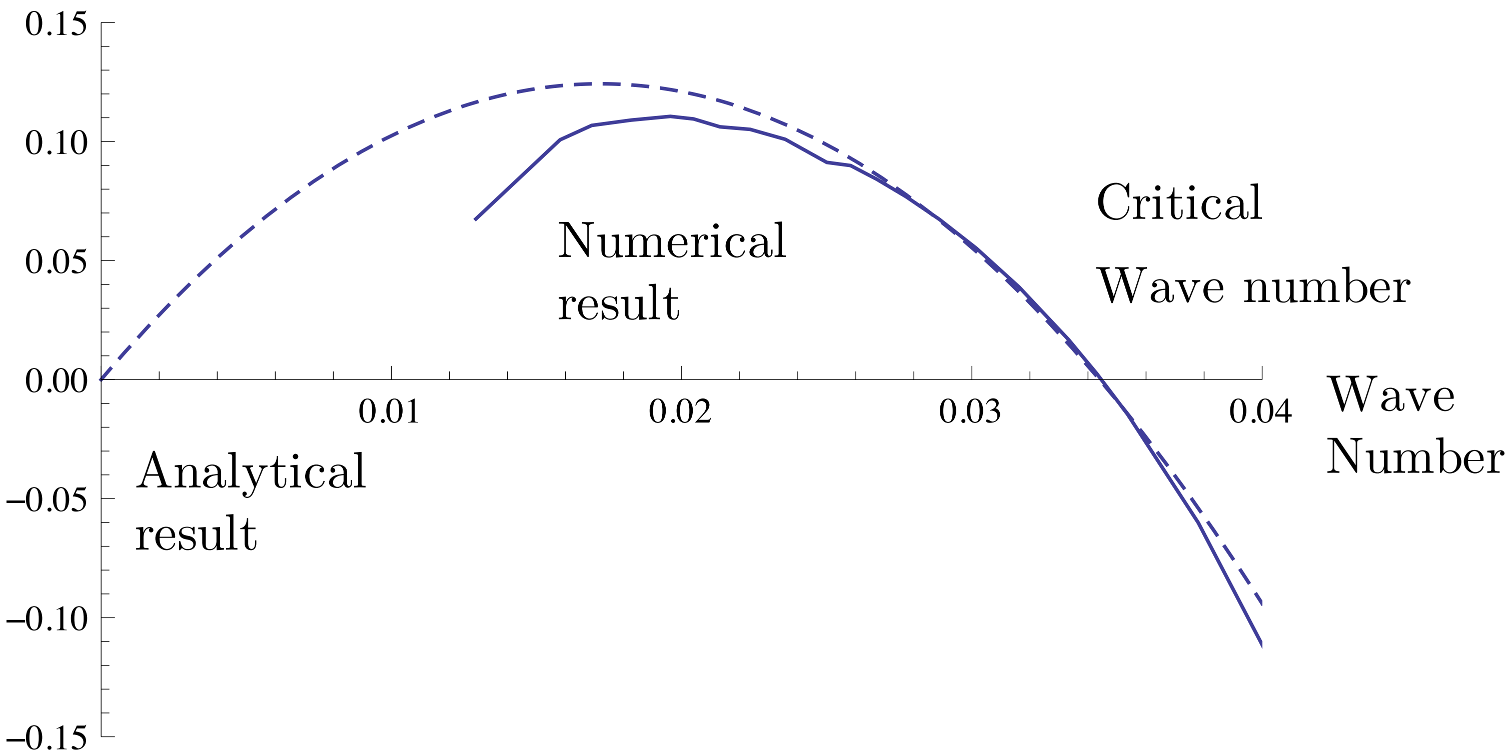
<u>Fluid</u>

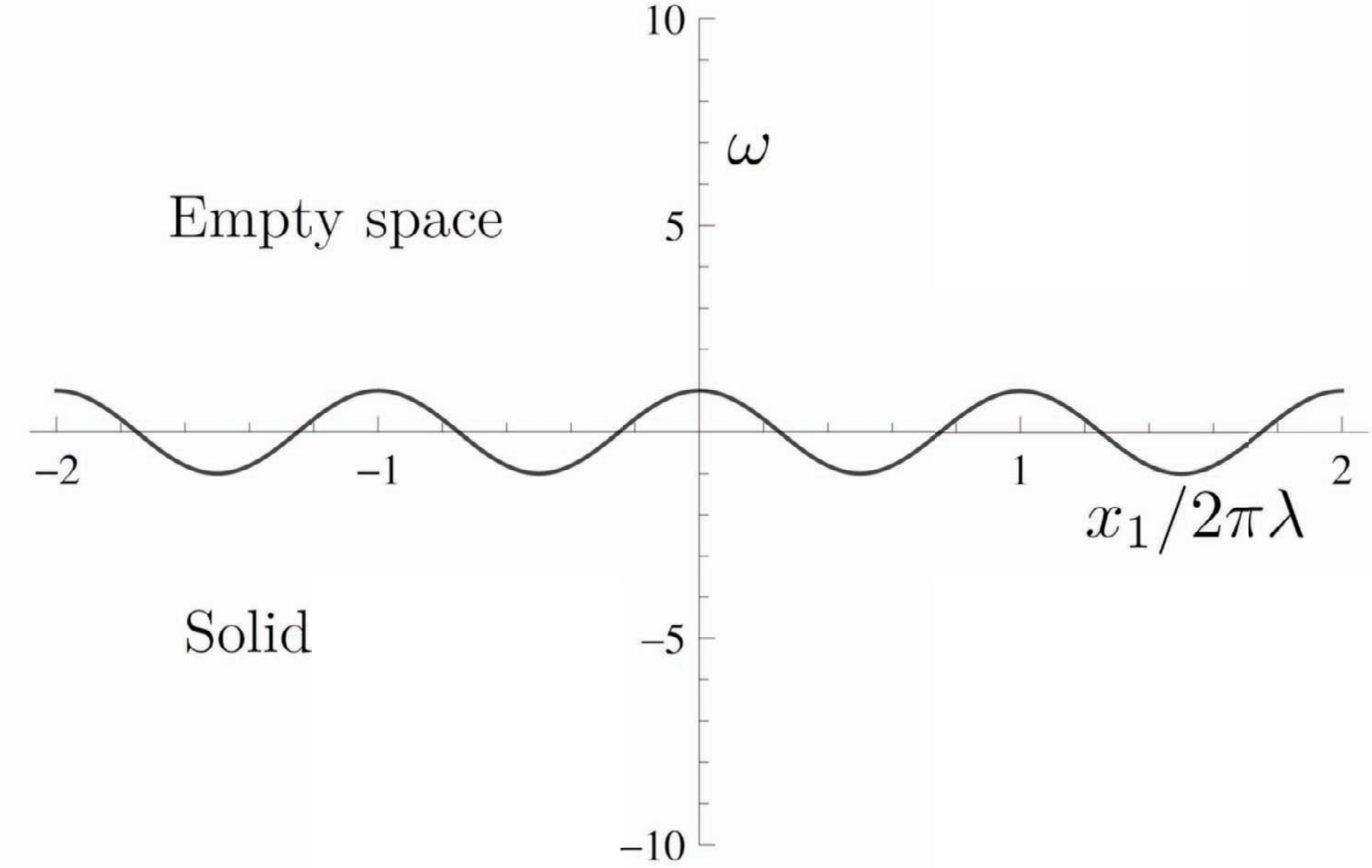
$$h_{,t} = k[(\mu/2)\varepsilon_o\,\omega - \gamma\omega^2]h$$



(verified by Kim et al., 2000)

Relative Growth Rate




10
5
−5
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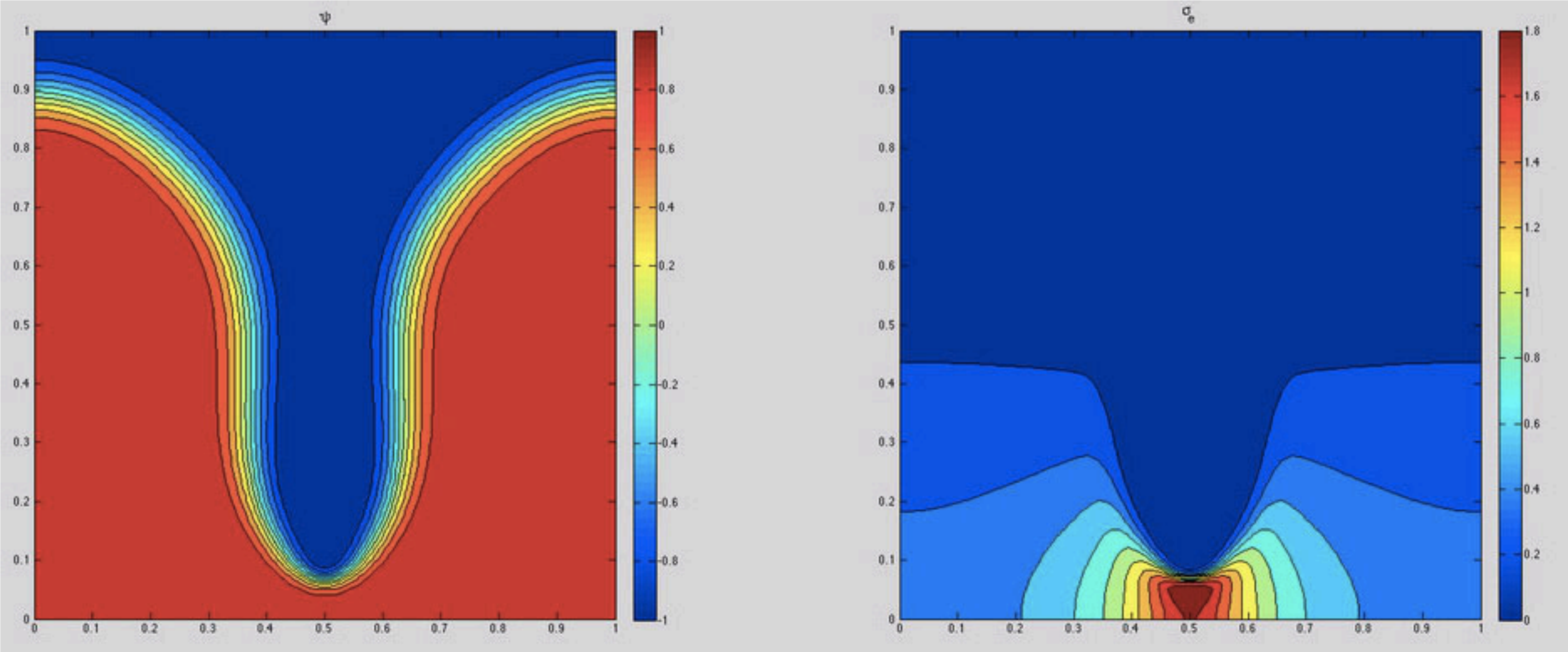
ω
Empty space
Solid
−2
−1
1
2
$x_1/2\pi\lambda$


ψ
σ_e
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0.4
0.5
0.6
0.7
0.8
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1
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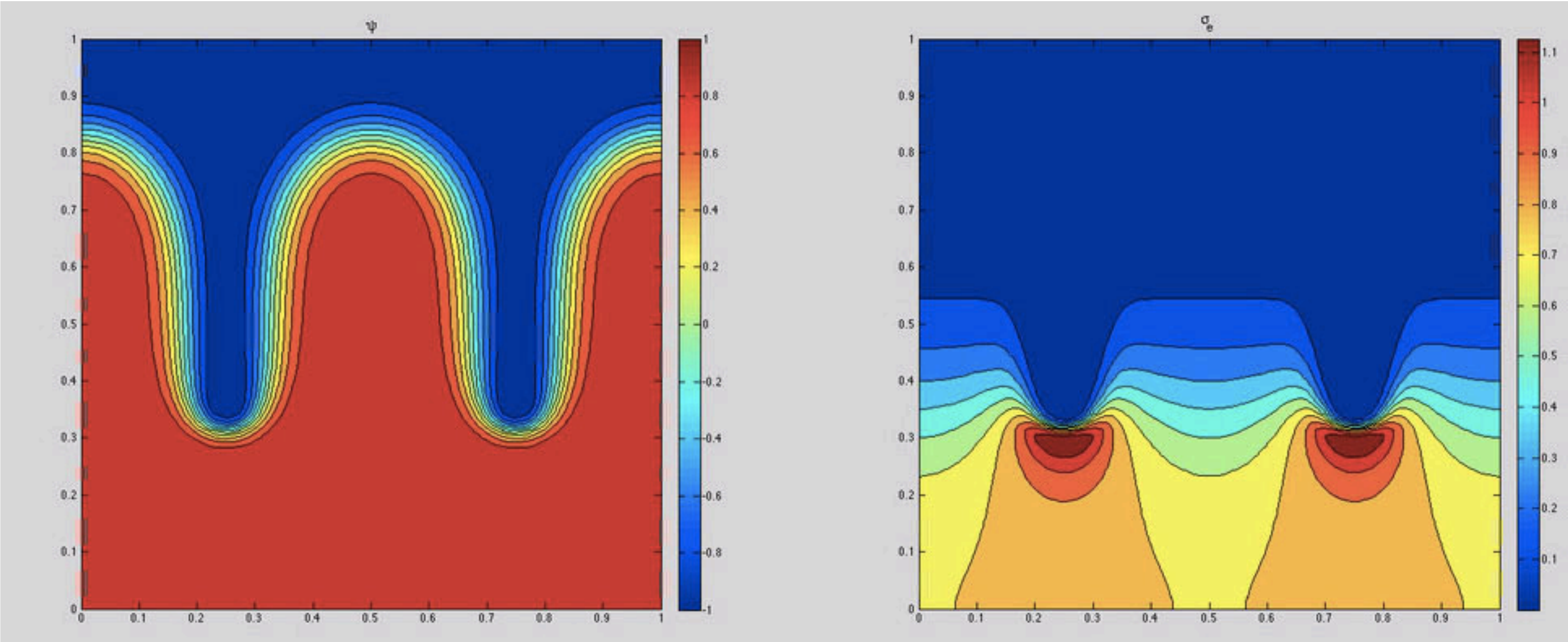
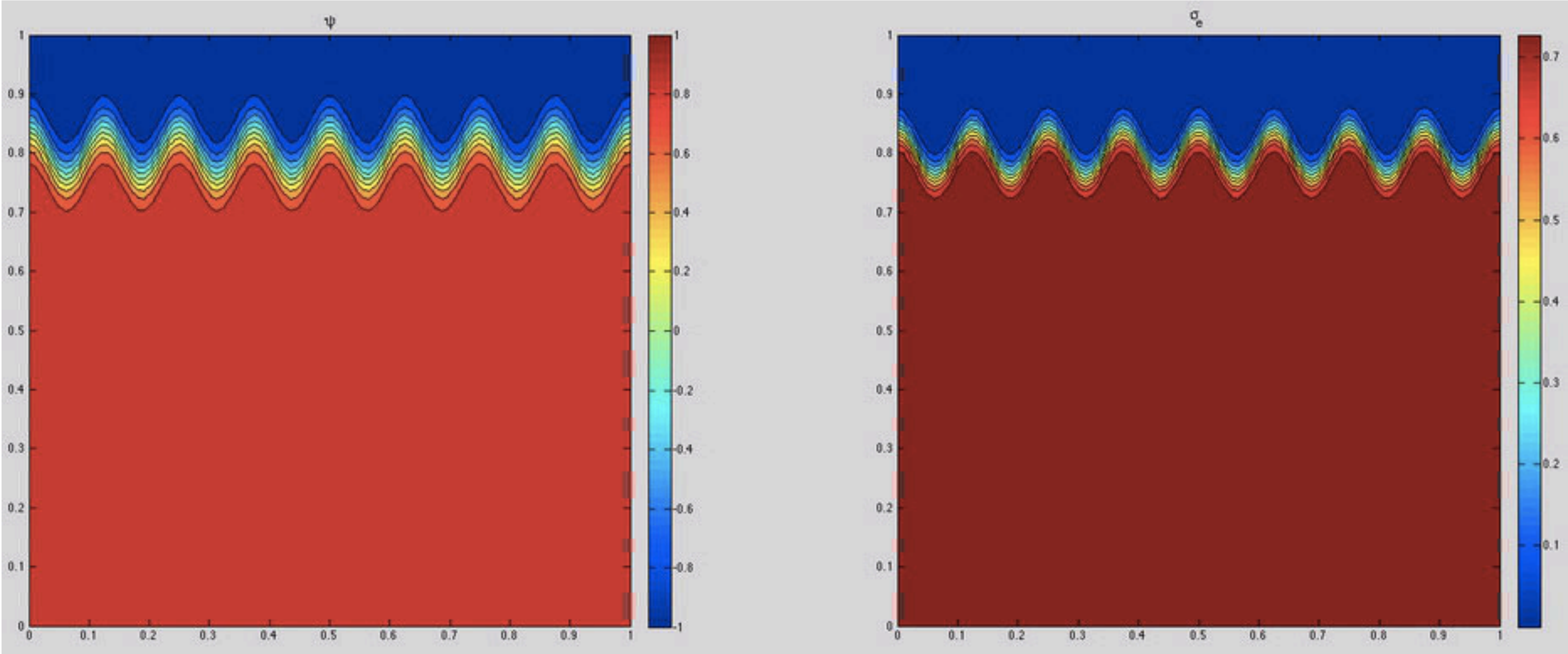
-0.8
-0.6
-0.4
-0.2
1.2
1.4
1.6
1.8


ψ
σe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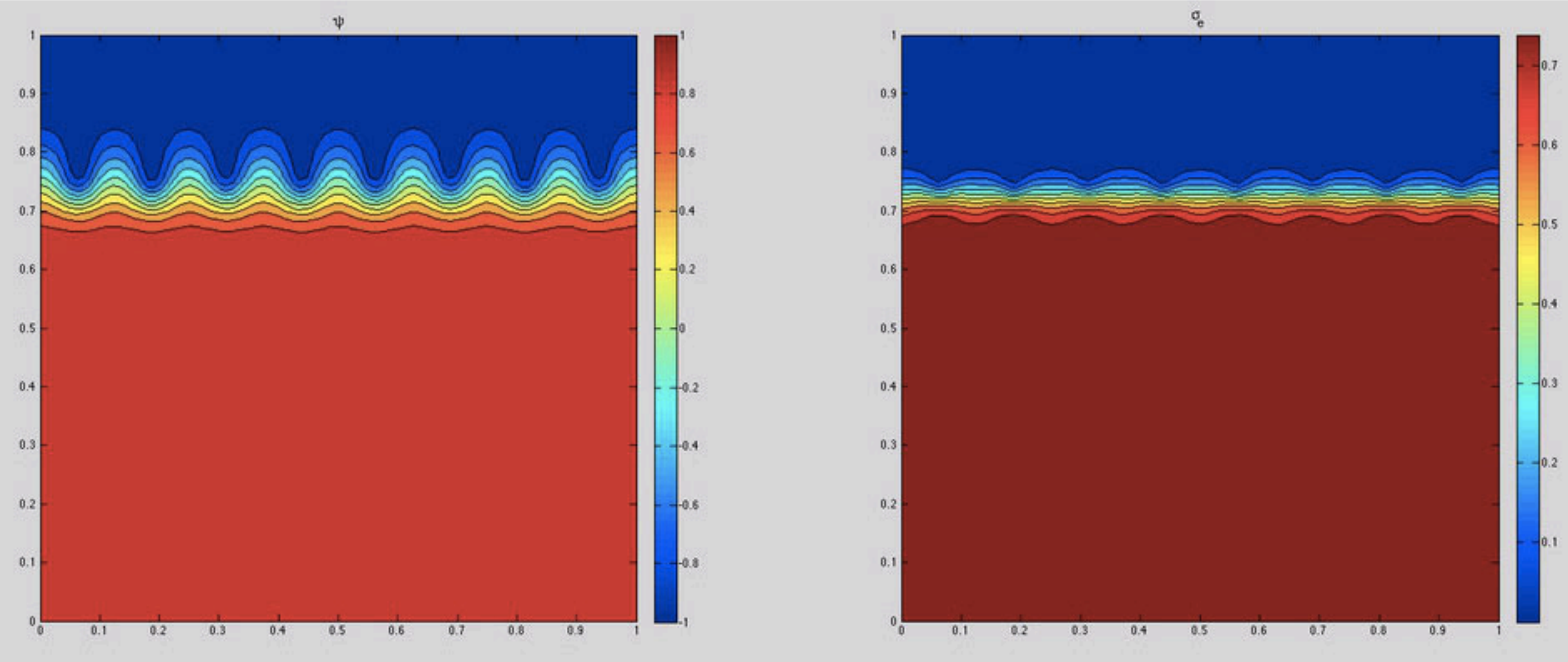
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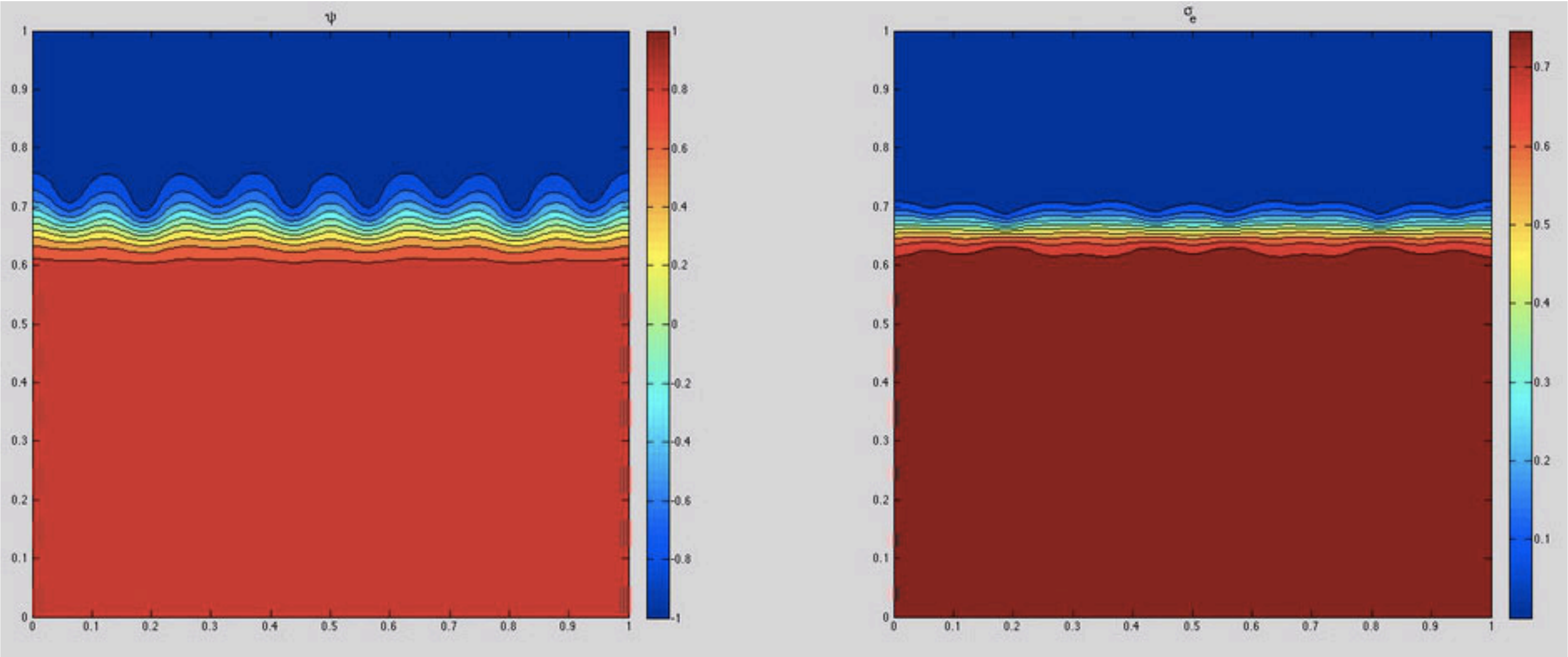
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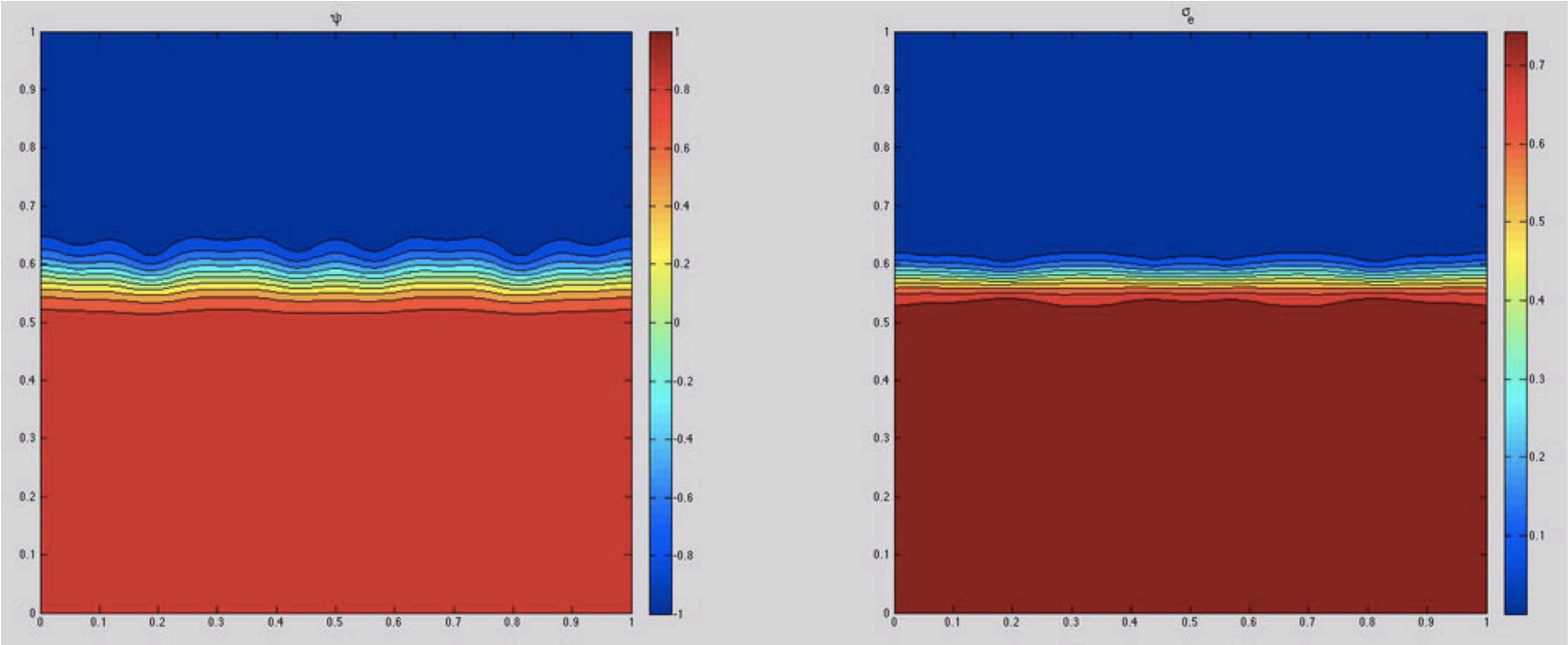
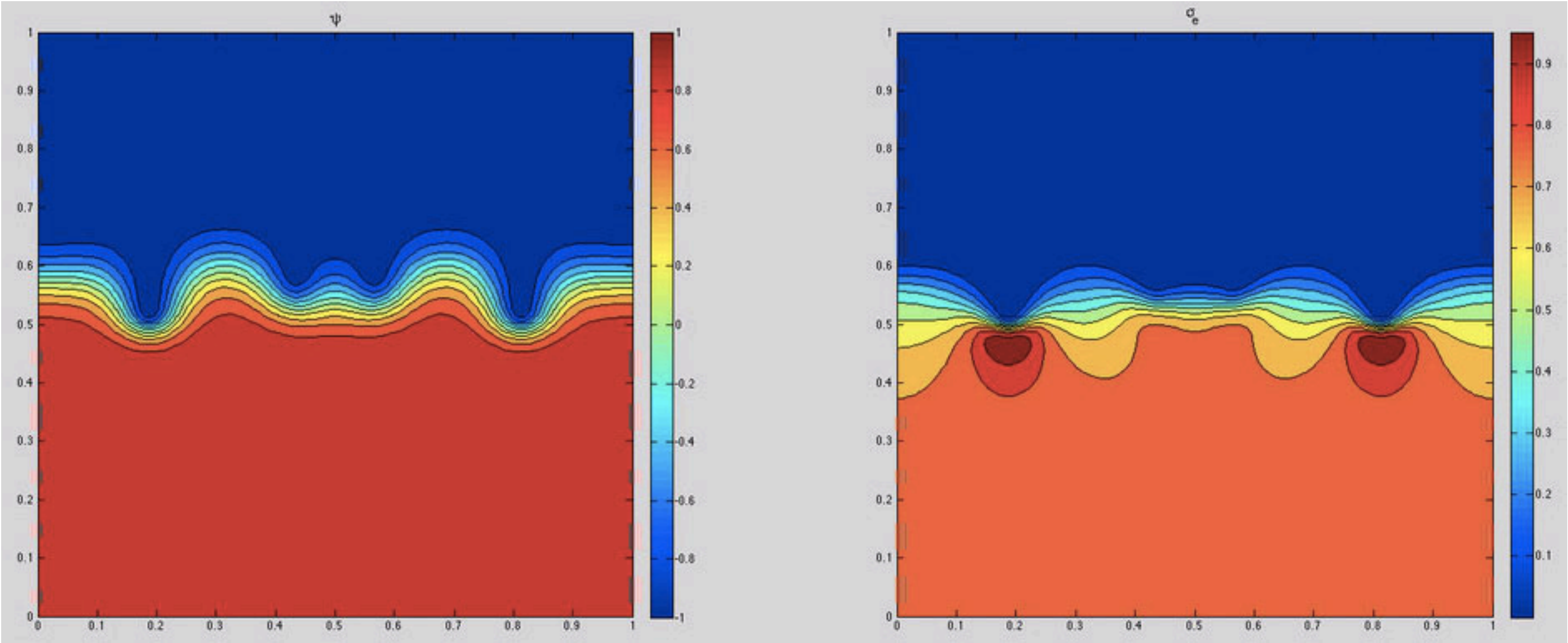


ψ
σ_e



ψ
σ_e
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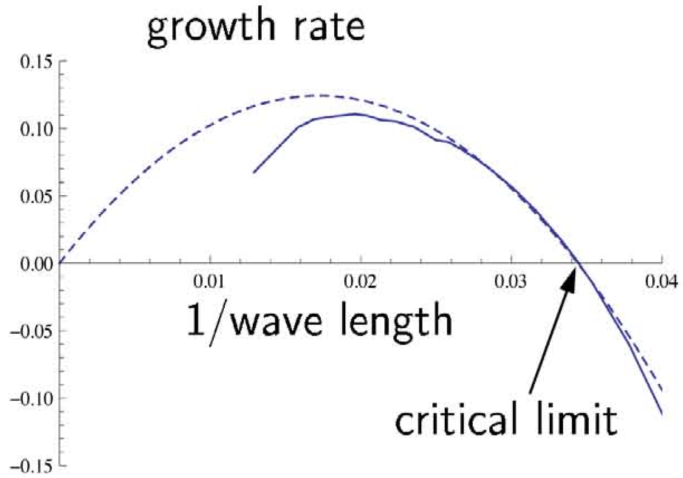
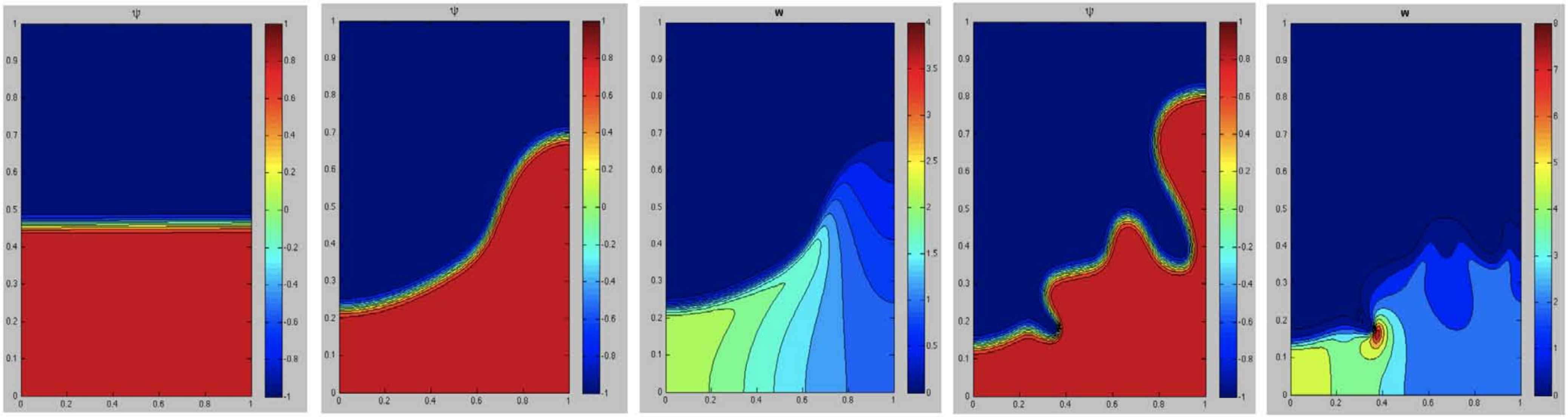
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
-1
-0.8
-0.6
-0.4
-0.2
0.2
0.4
0.6
0.8

$$(\frac{\mathrm{d}}{\mathrm{d}x_2} - 2\beta)(f' + f^2 - 1) = 0$$



$$\psi = -\tanh(\sqrt{\frac{p}{2g_b}}x_2 + \frac{3}{4}L_\psi G_o(\nabla w)^2\sqrt{\frac{2g_b}{p}}t)$$

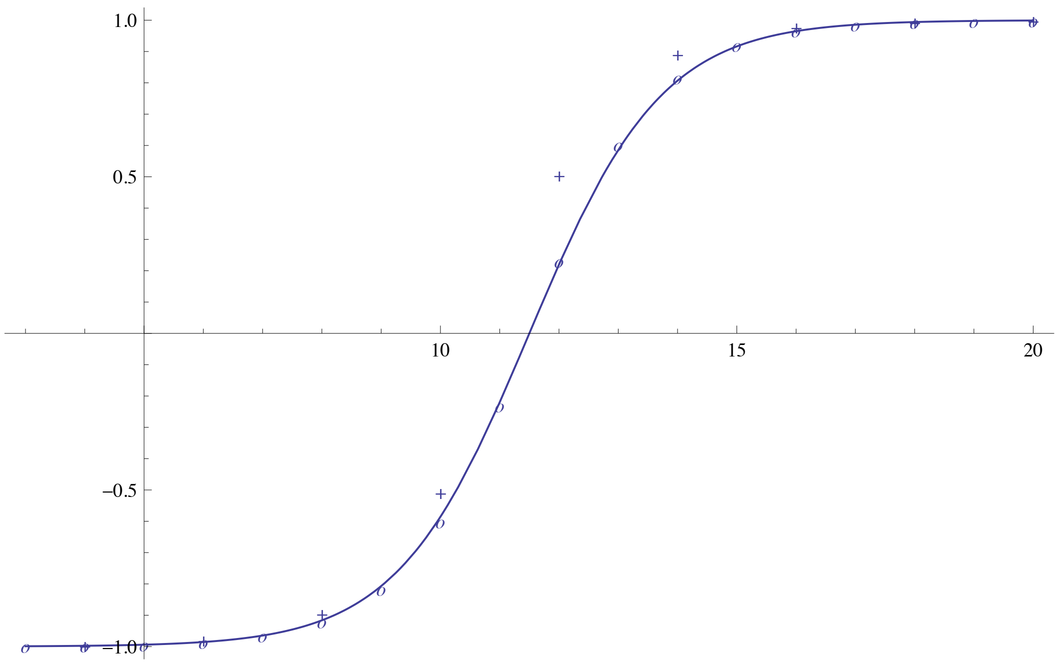


Red is remaining material Effective Stress Effective Stress

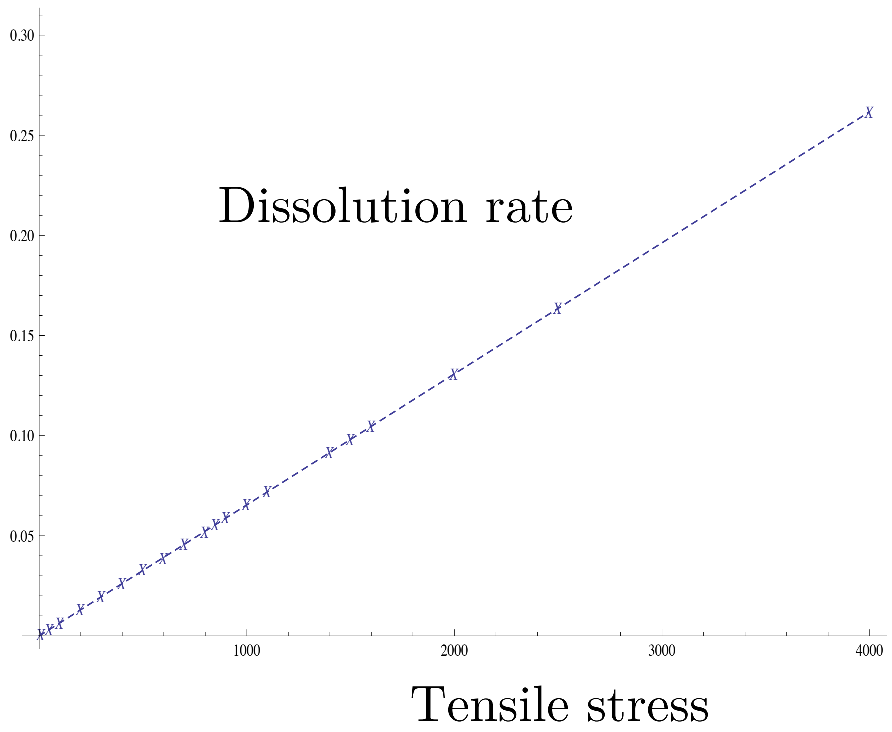
Steady state solution

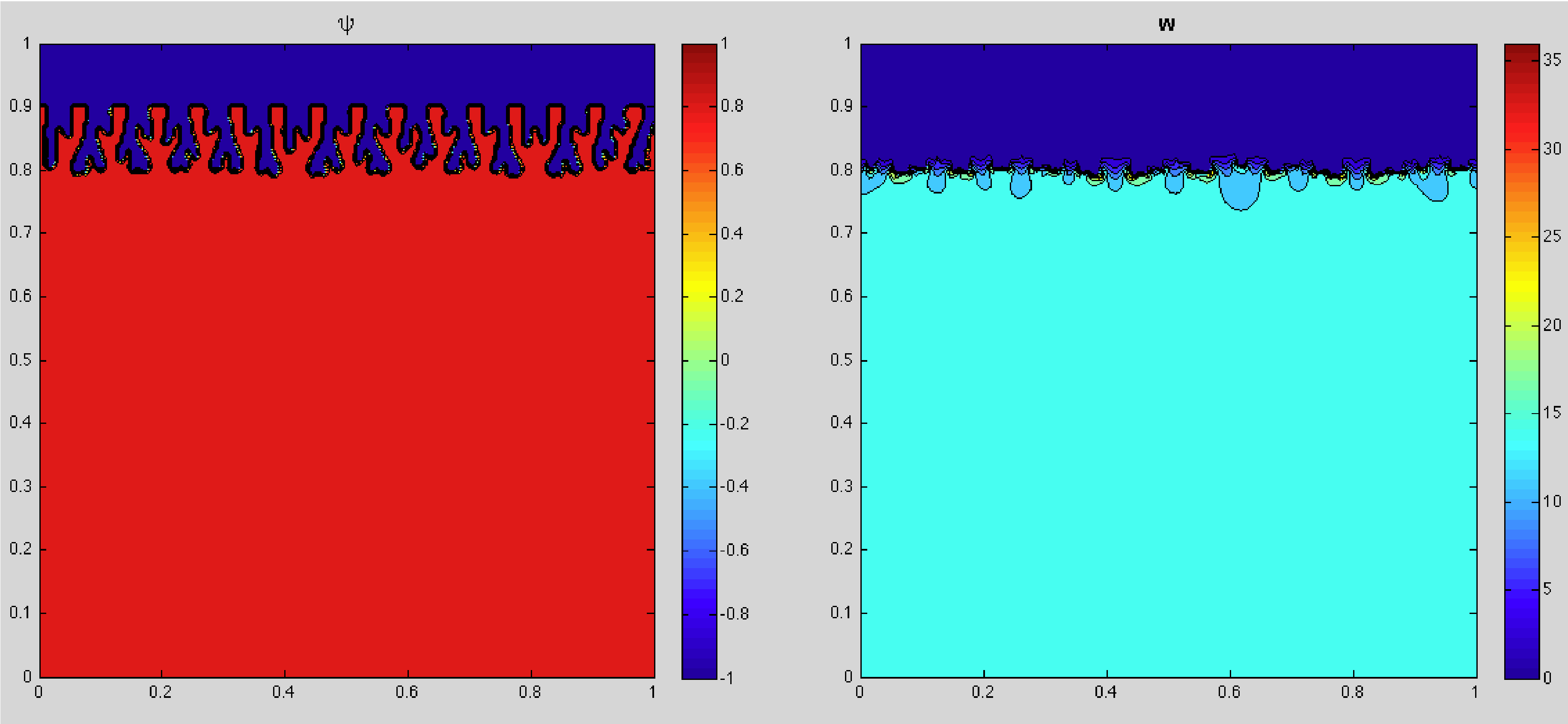
$$\psi = -\tanh\left(\sqrt{\frac{p}{2g_b}}x_2 + \frac{3}{4}L_\psi G_o(\nabla w)^2\sqrt{\frac{2g_b}{p}}t\right)$$

Transition Rate vs. Distance



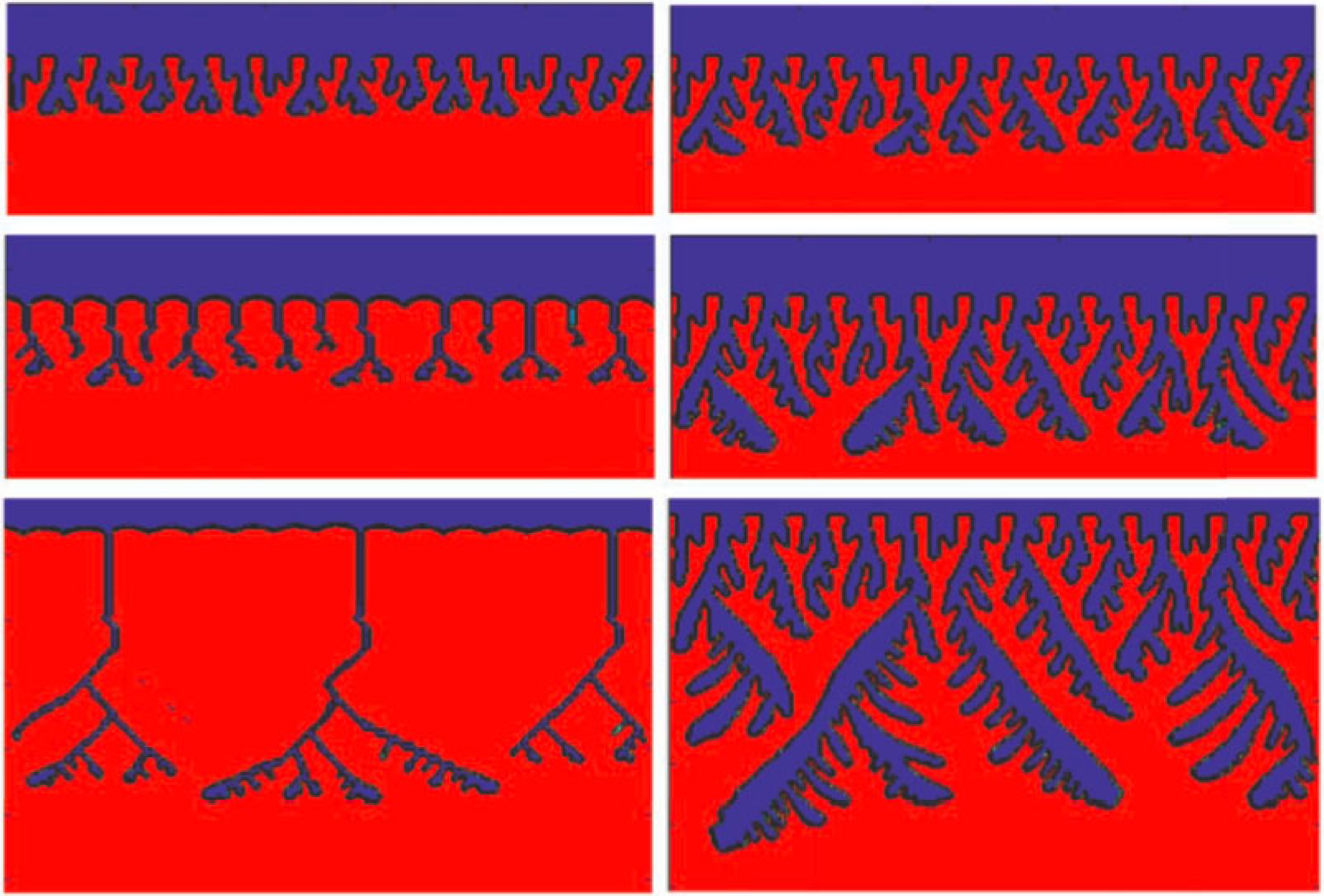
Dissolution Rate vs. Tensile Stress





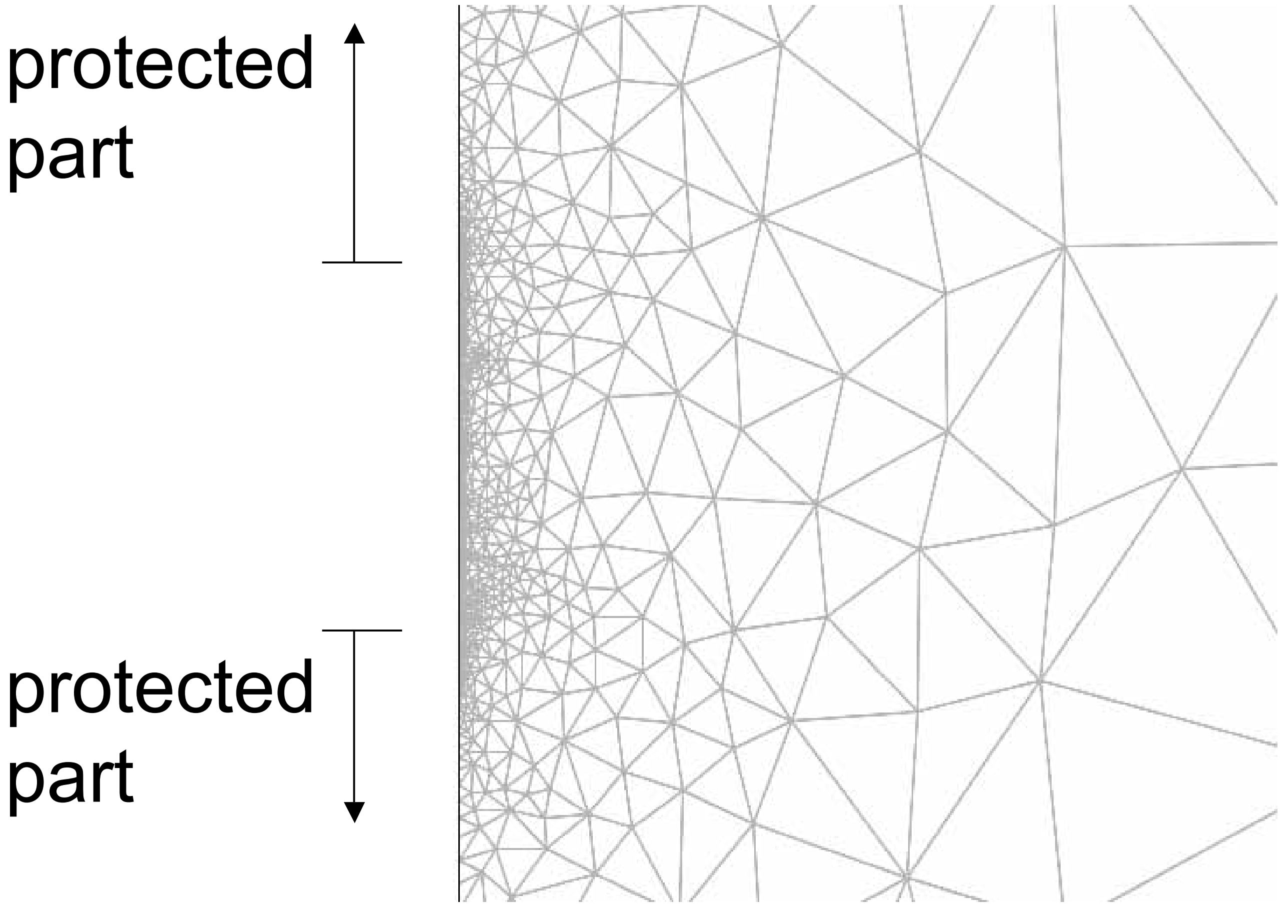
Red is remaining material

Effective stress

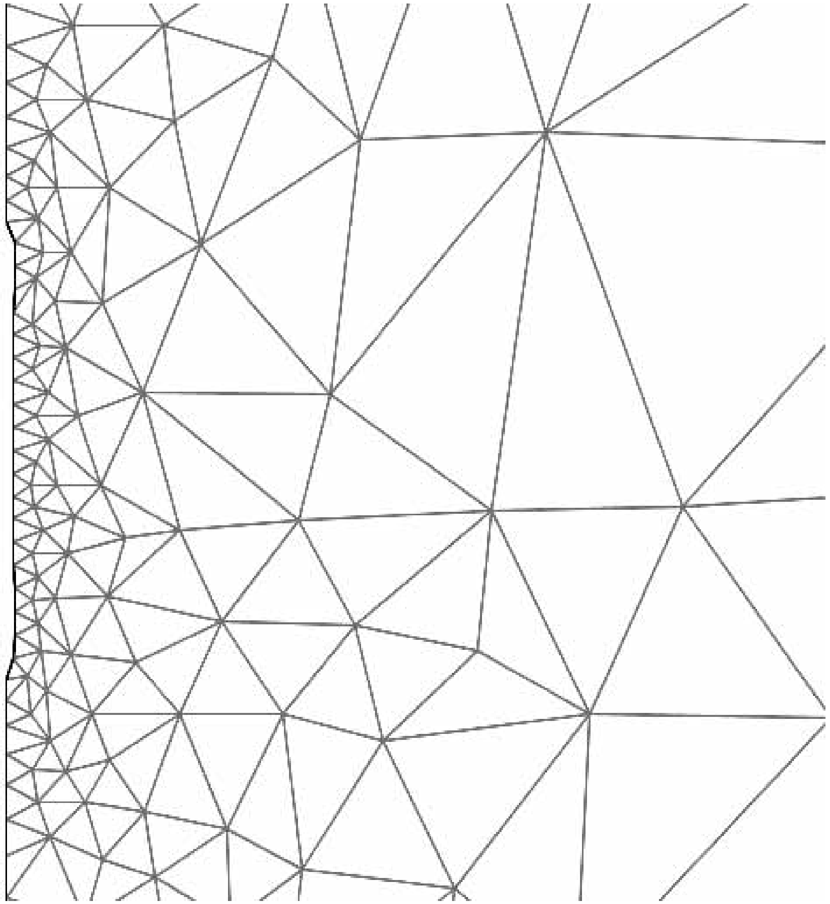


Without general corrosion with general corrosion

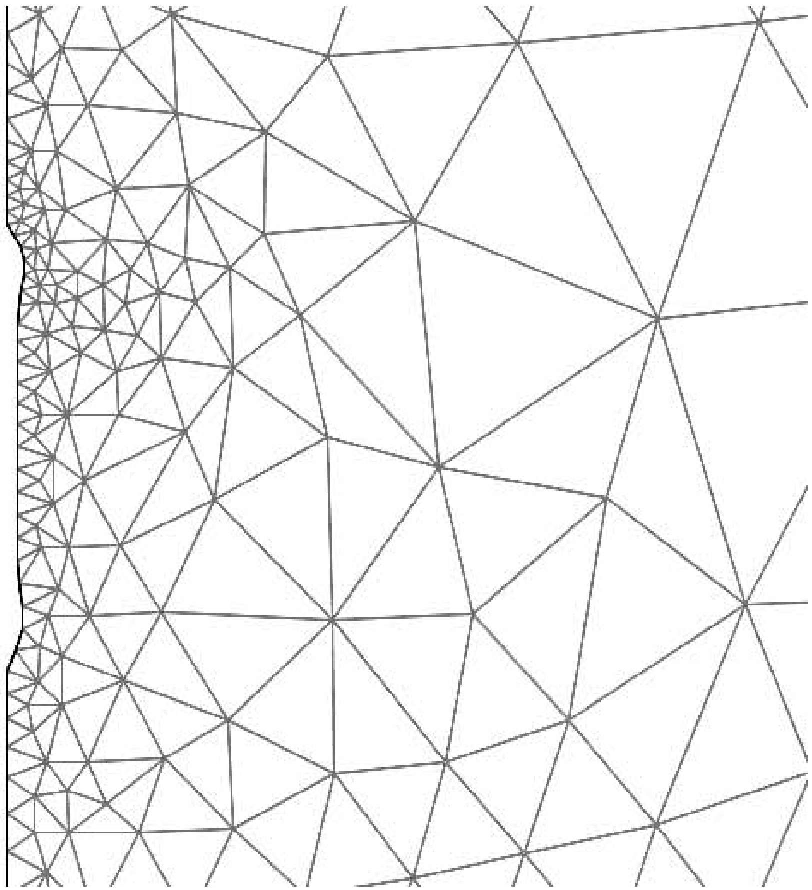
Corroding Surface



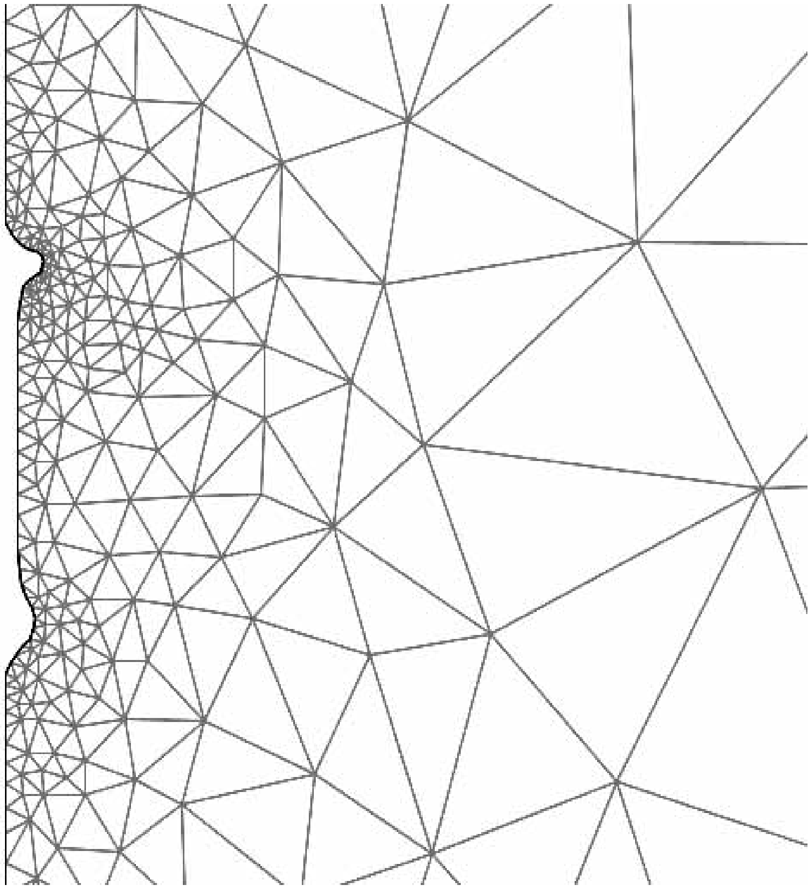
Corroding Surface



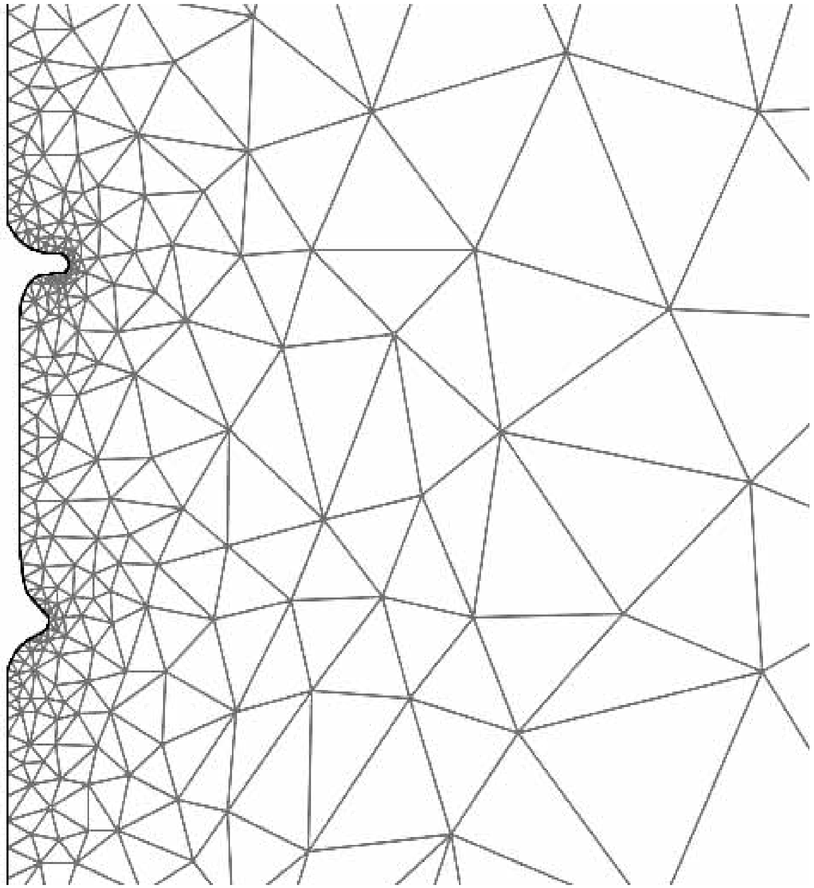
Corroding Surface



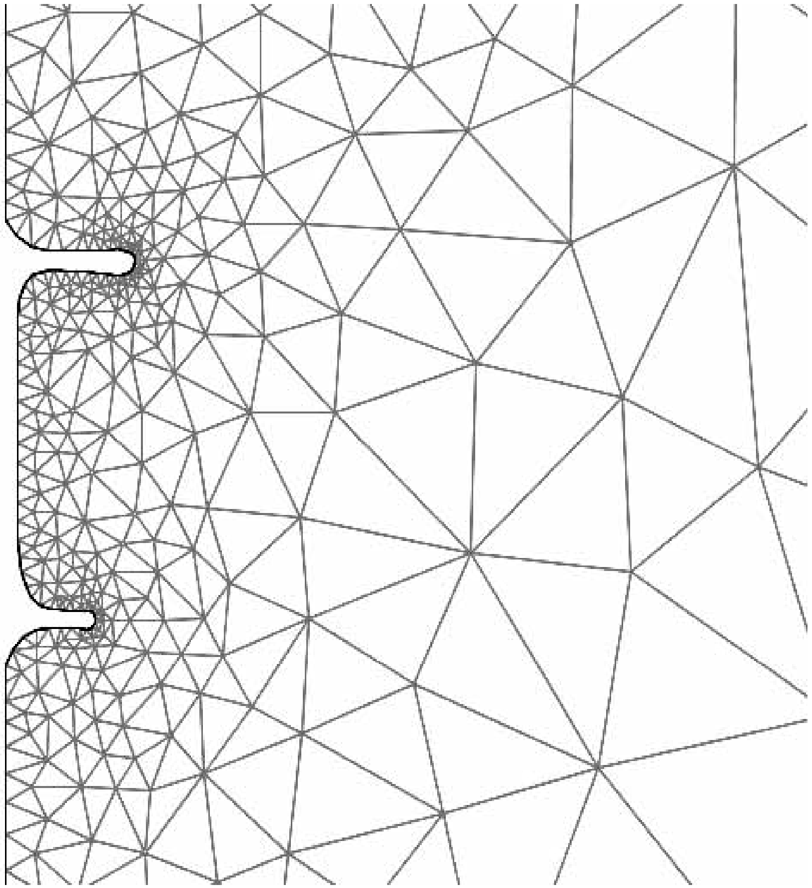
Corroding Surface



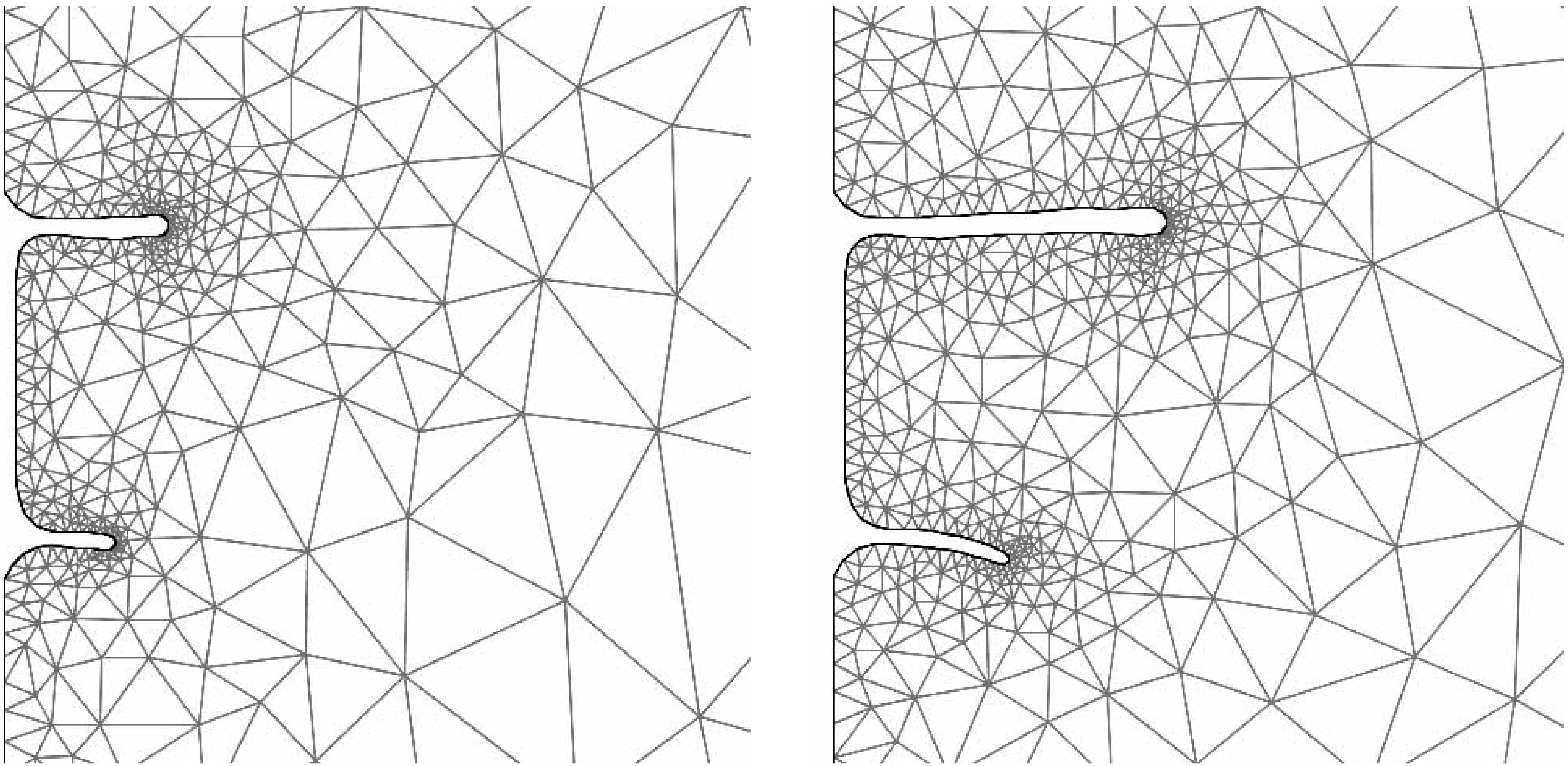
Corroding Surface



Corroding Surface

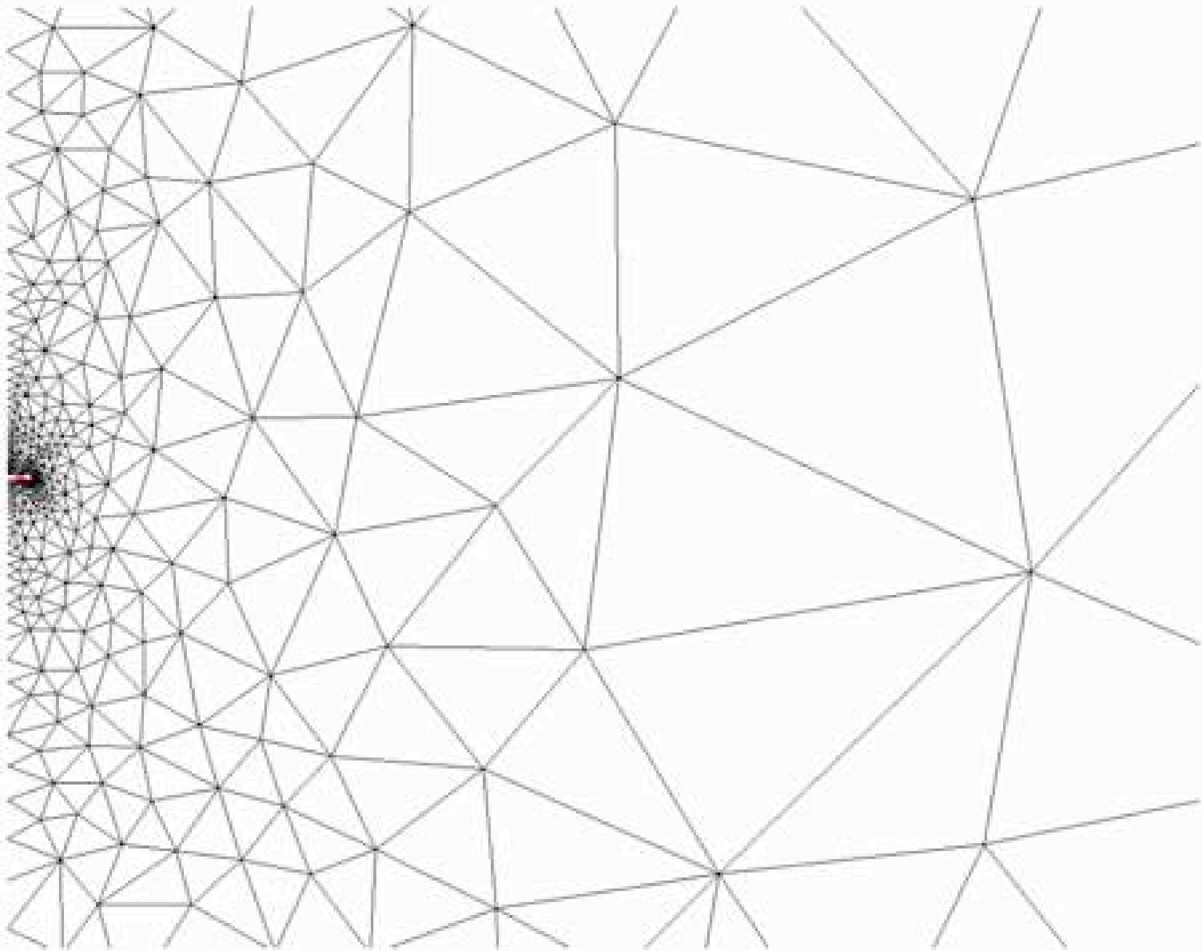


Corroding Surface



Branching

Branching



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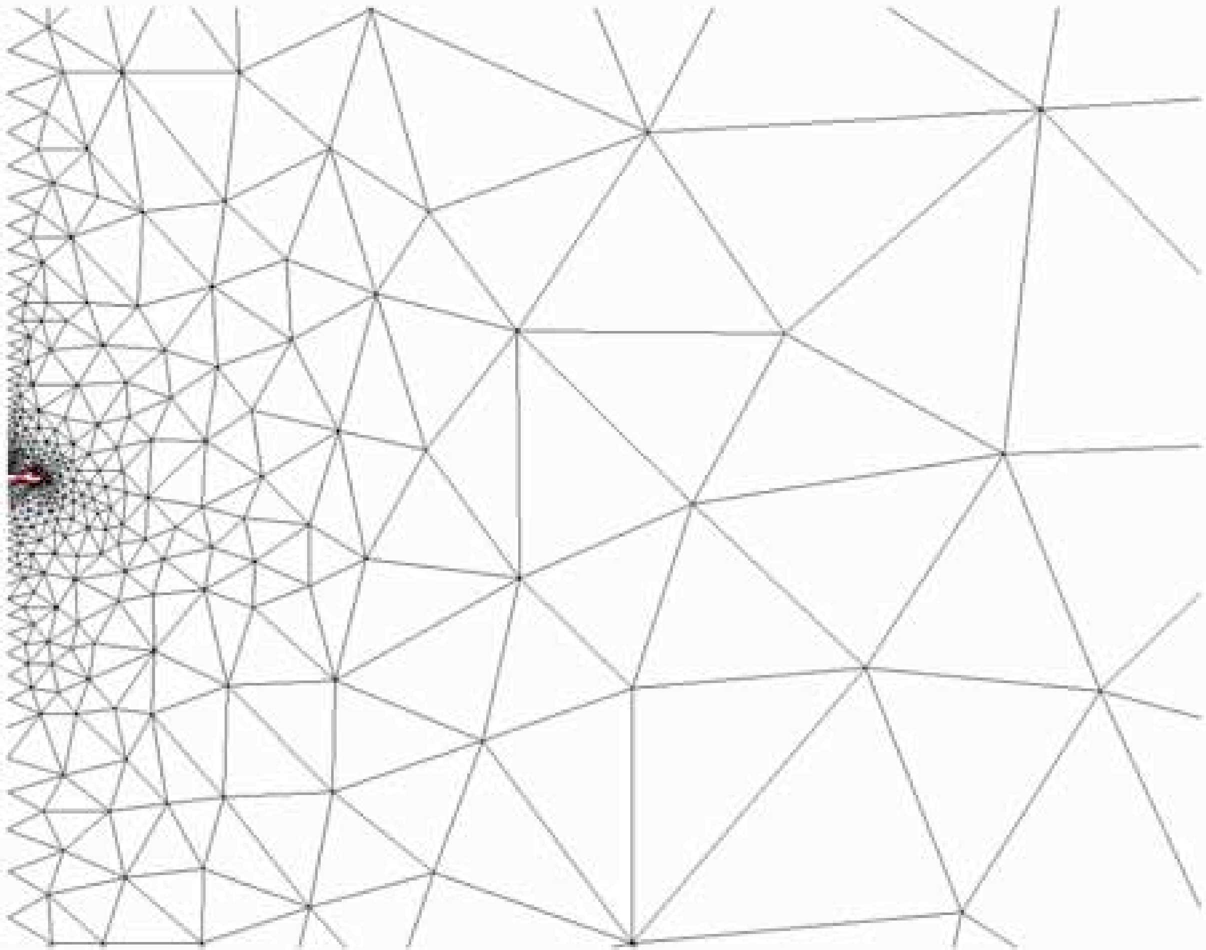

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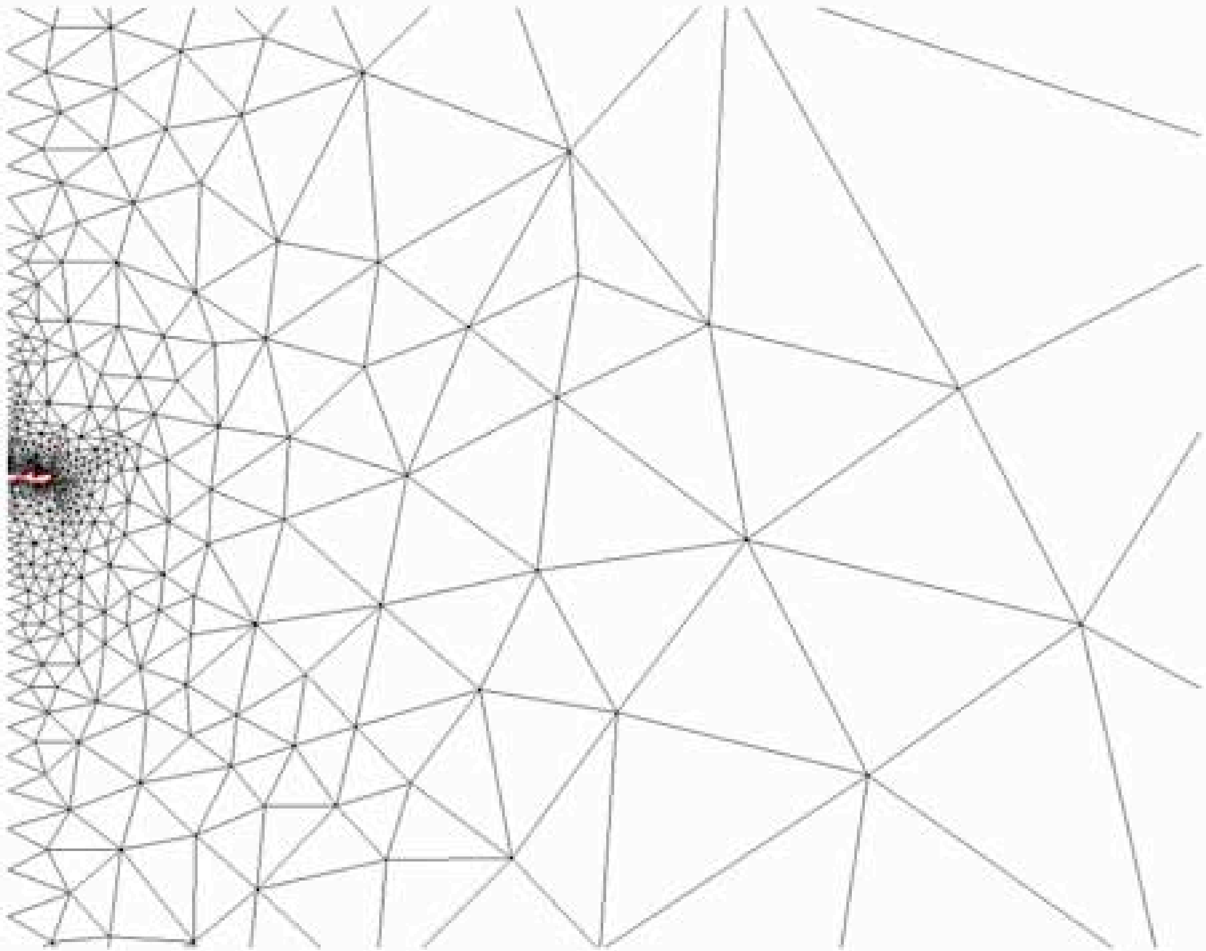

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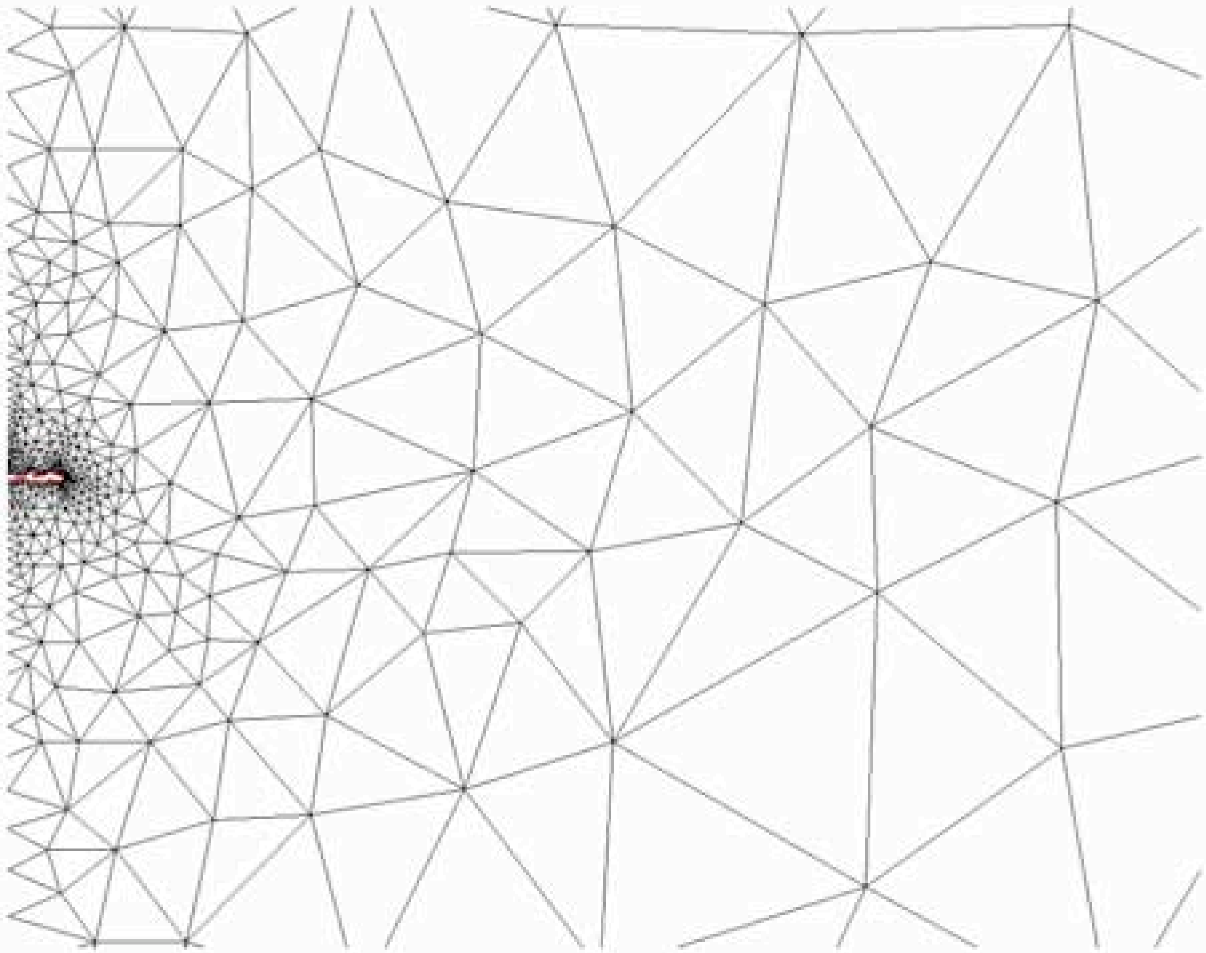

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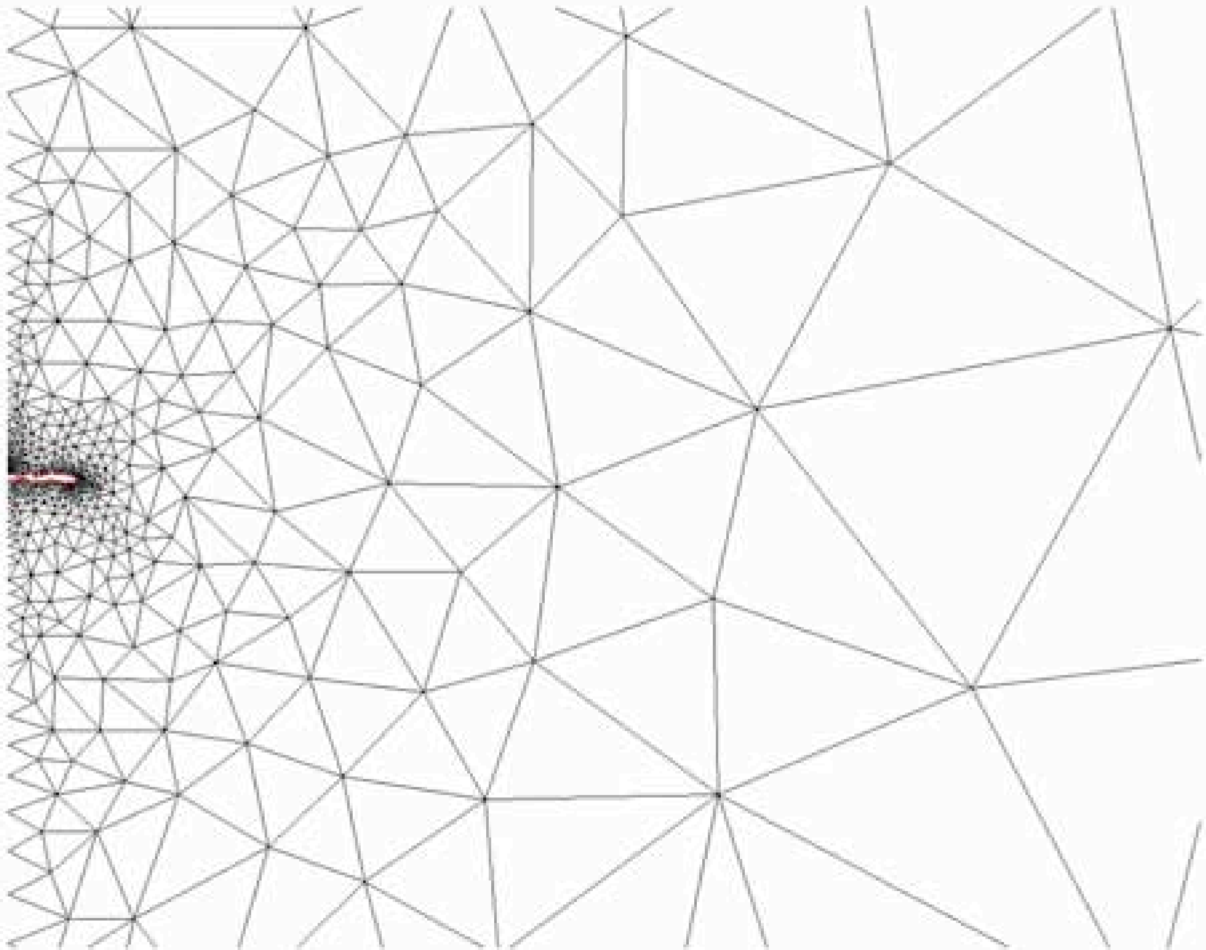

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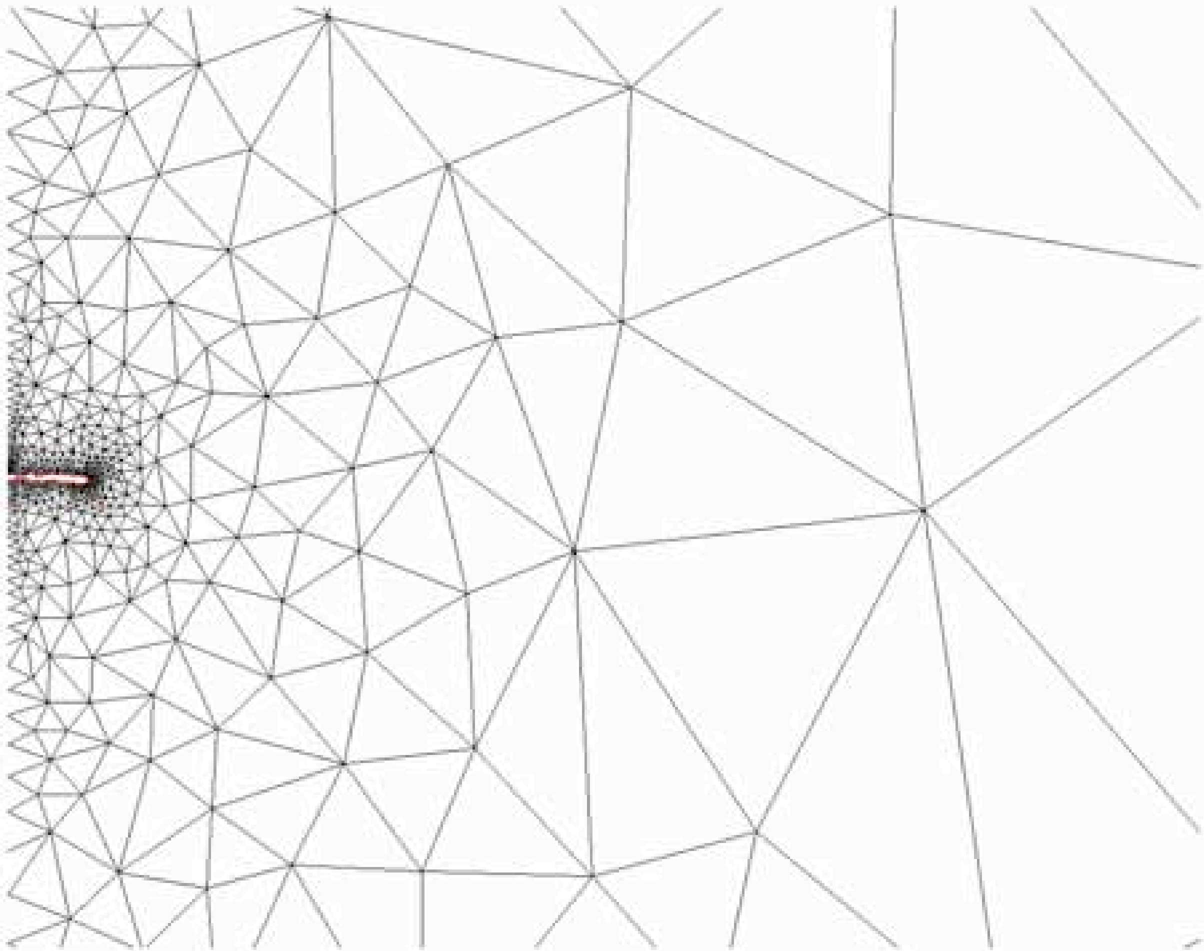

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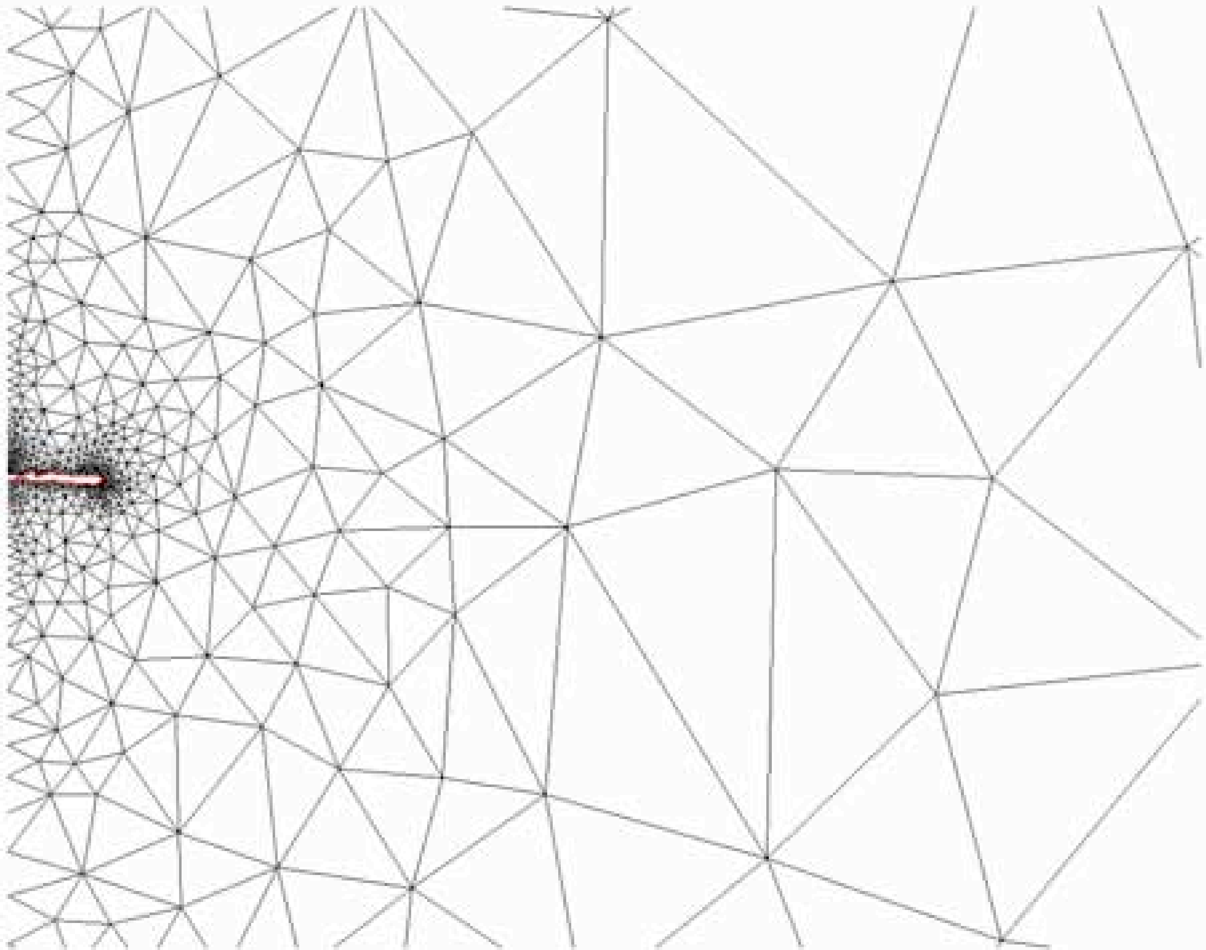

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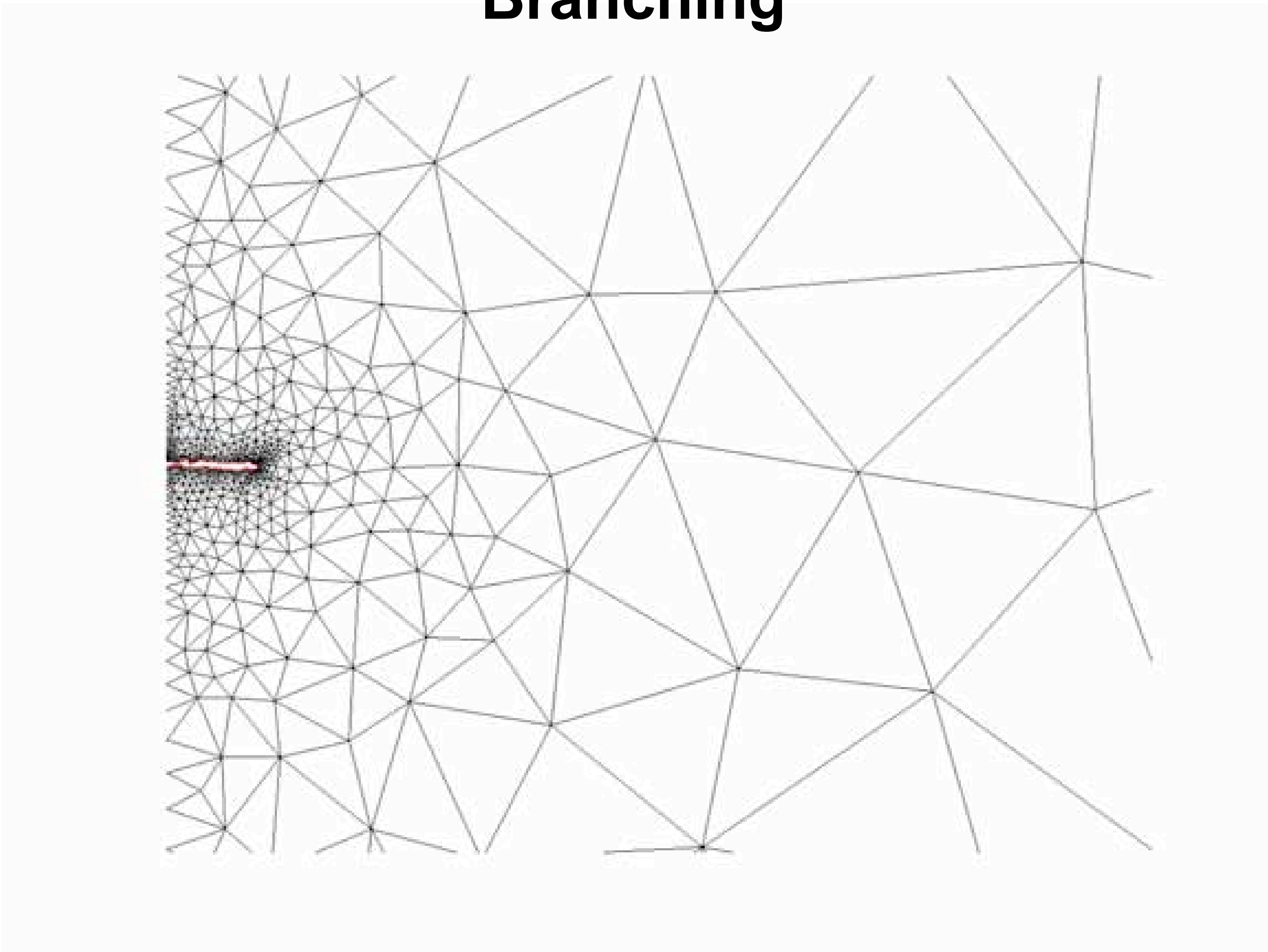

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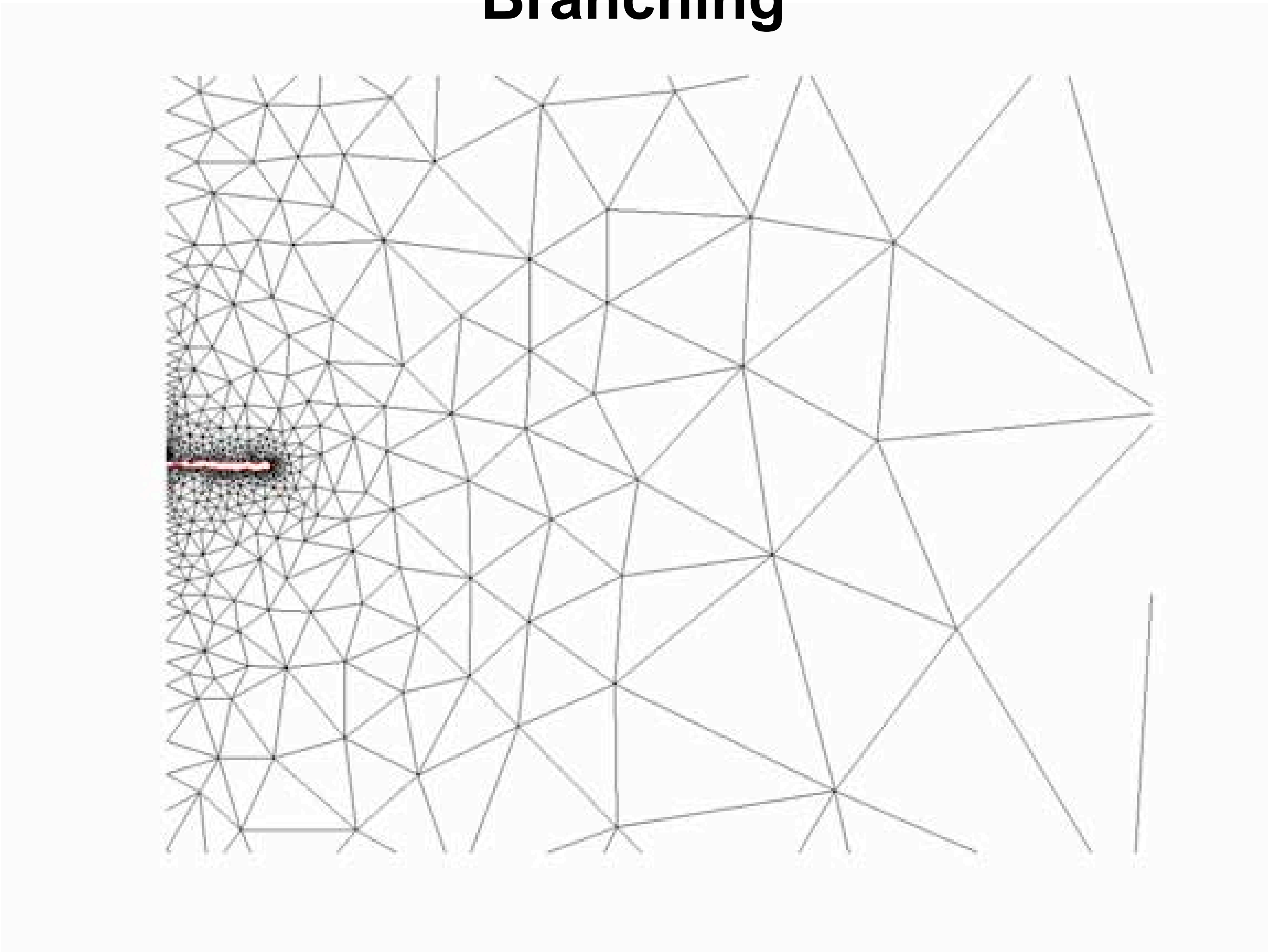

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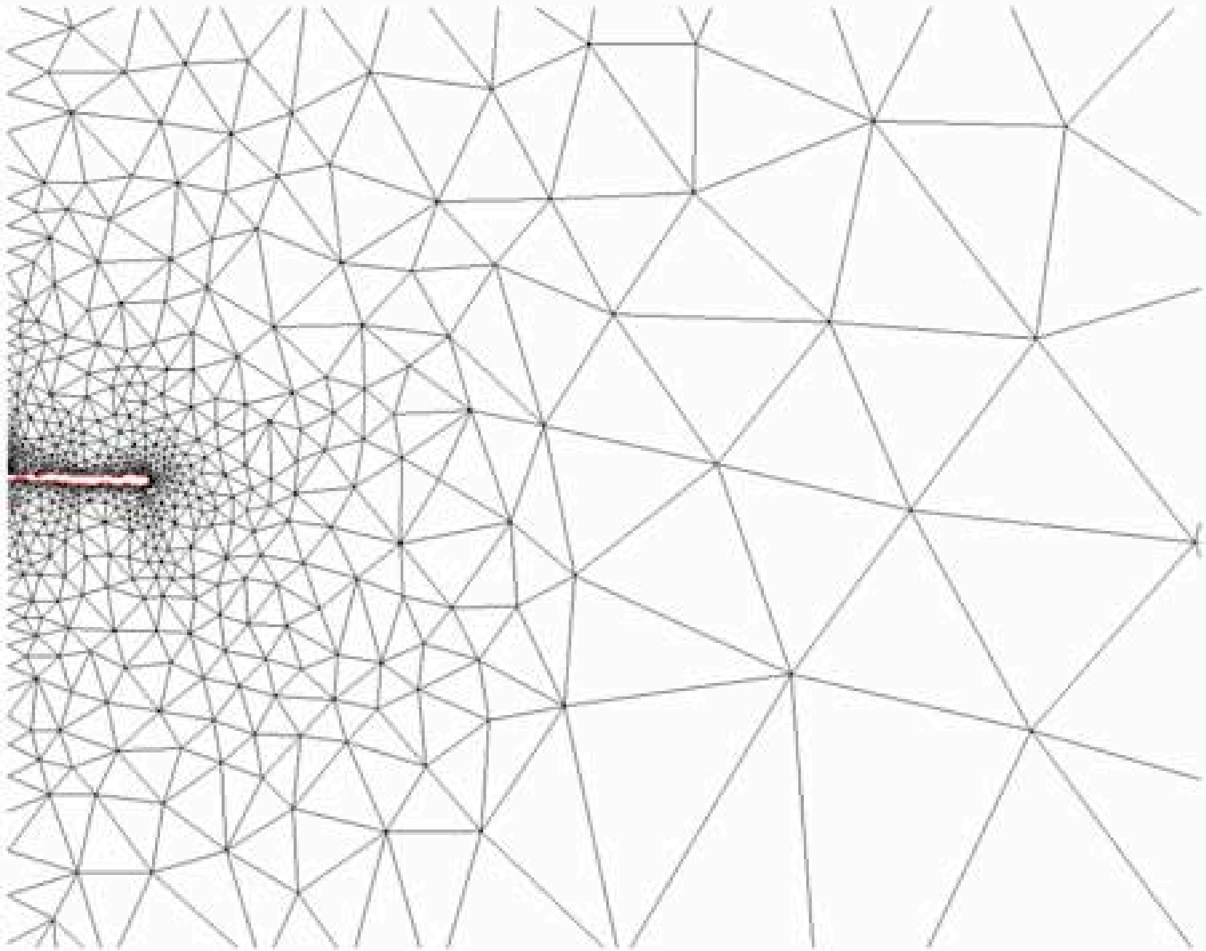

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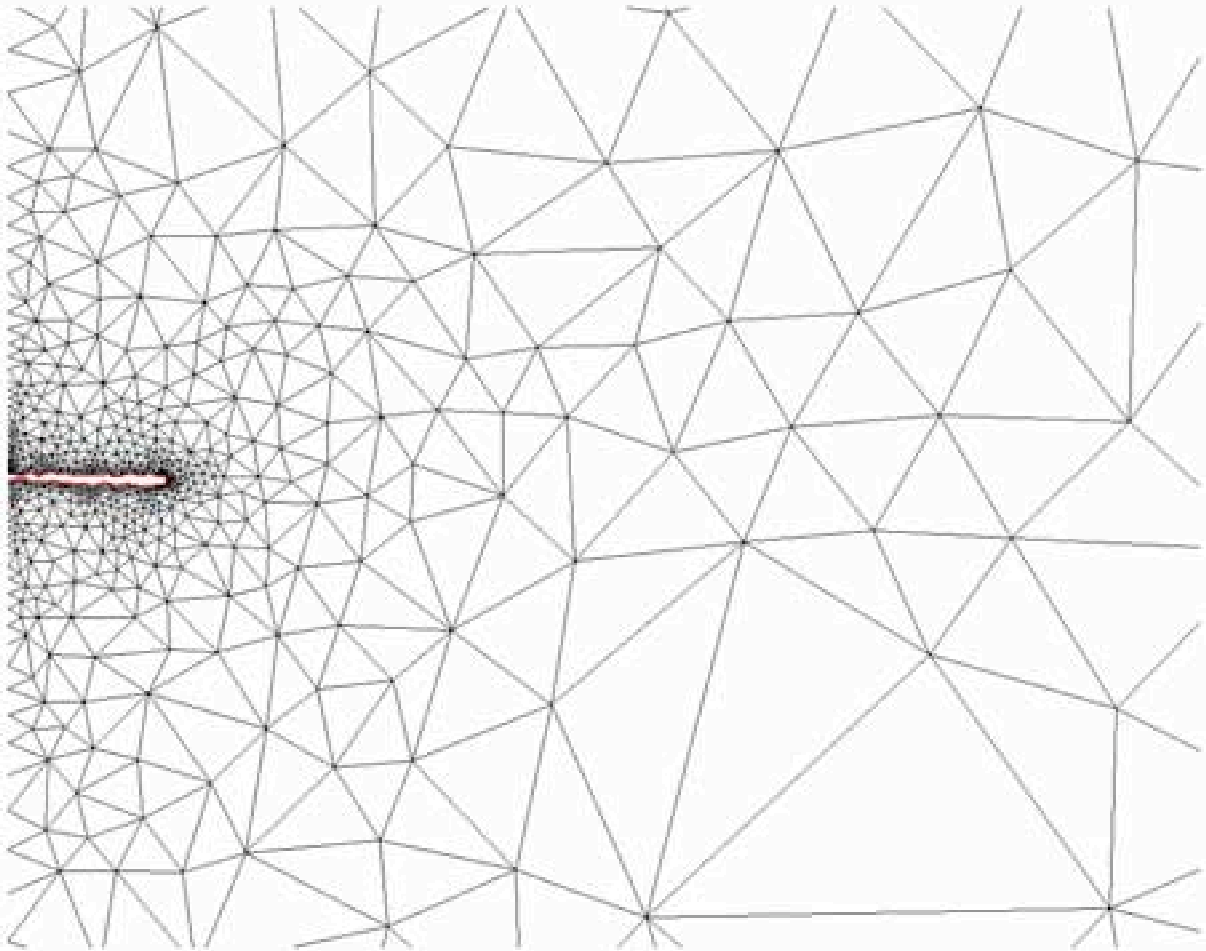

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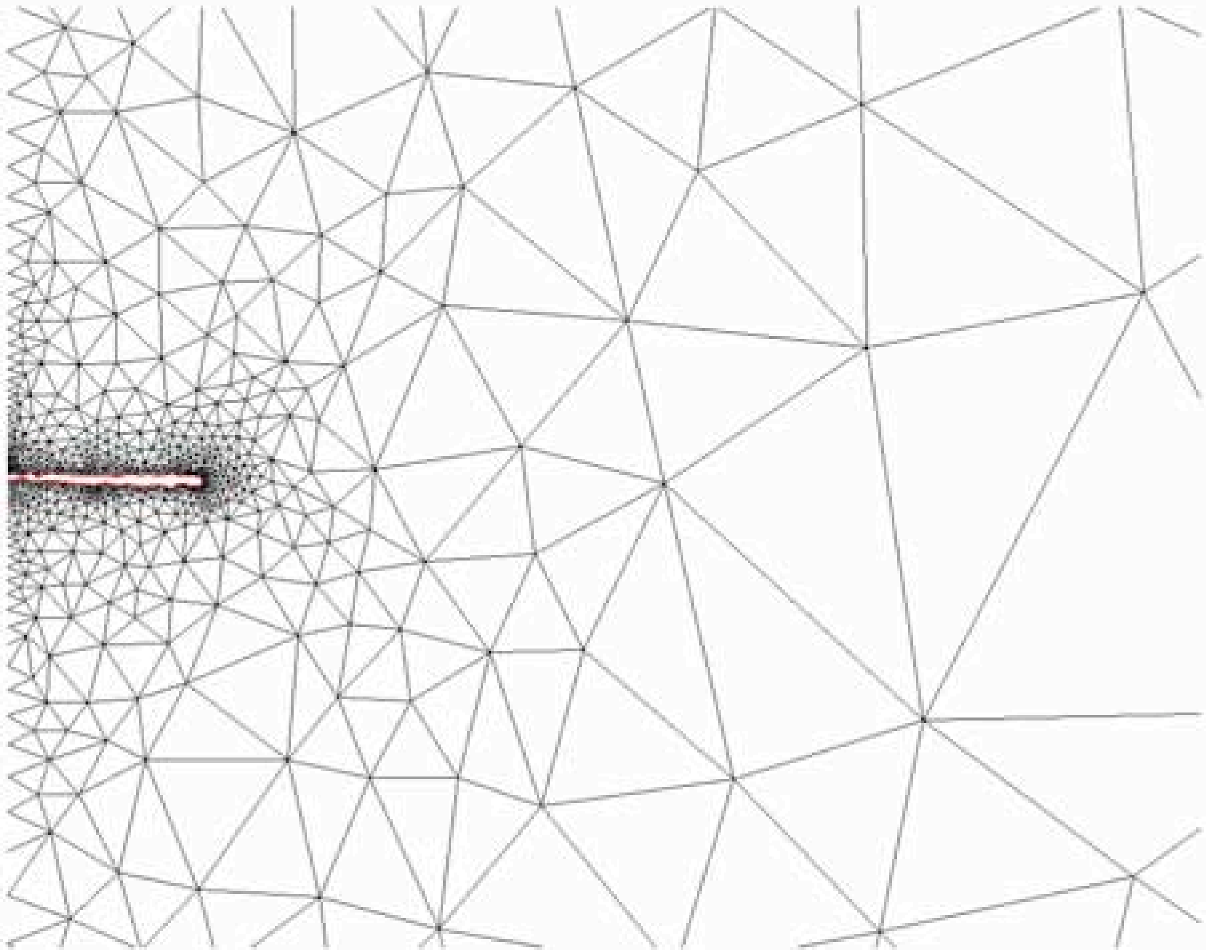

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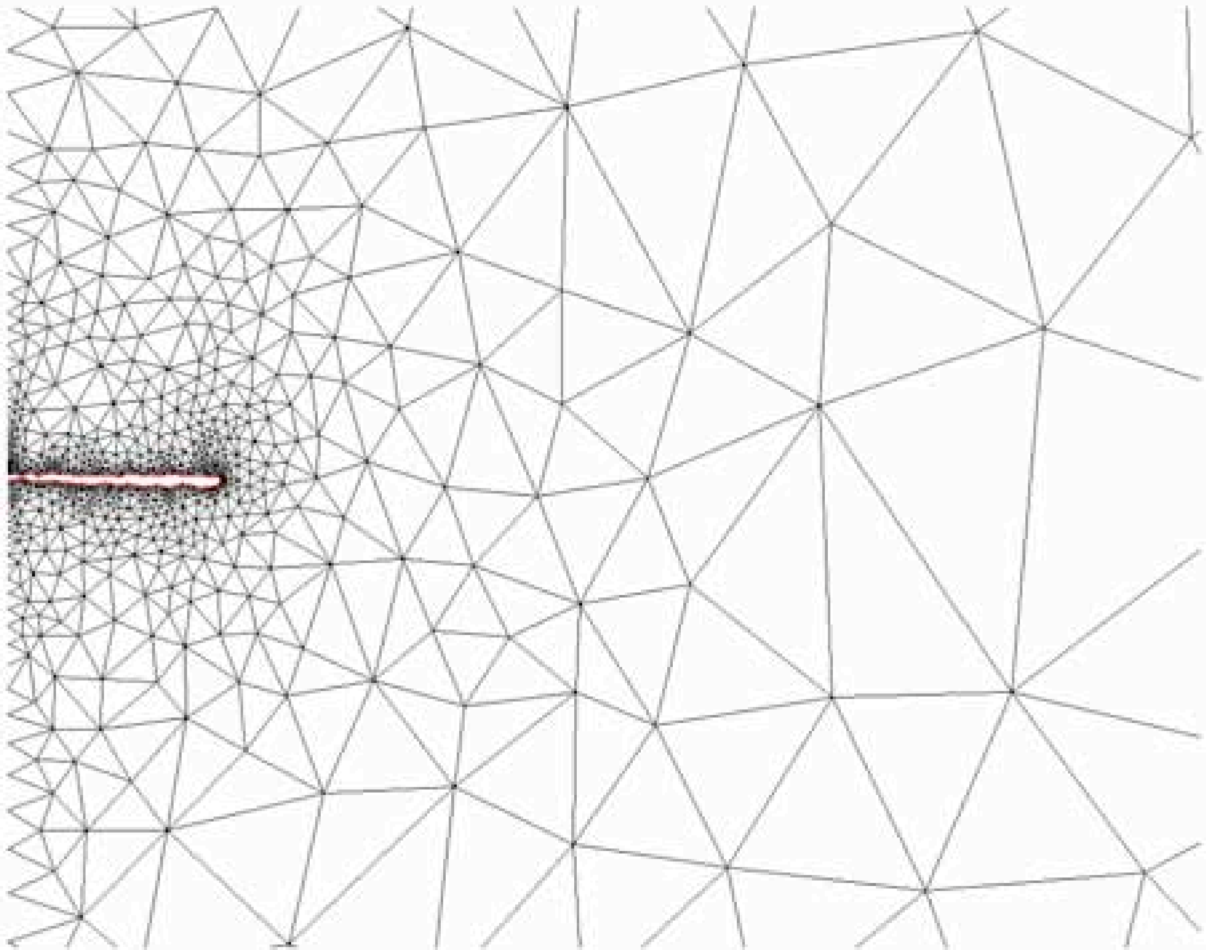

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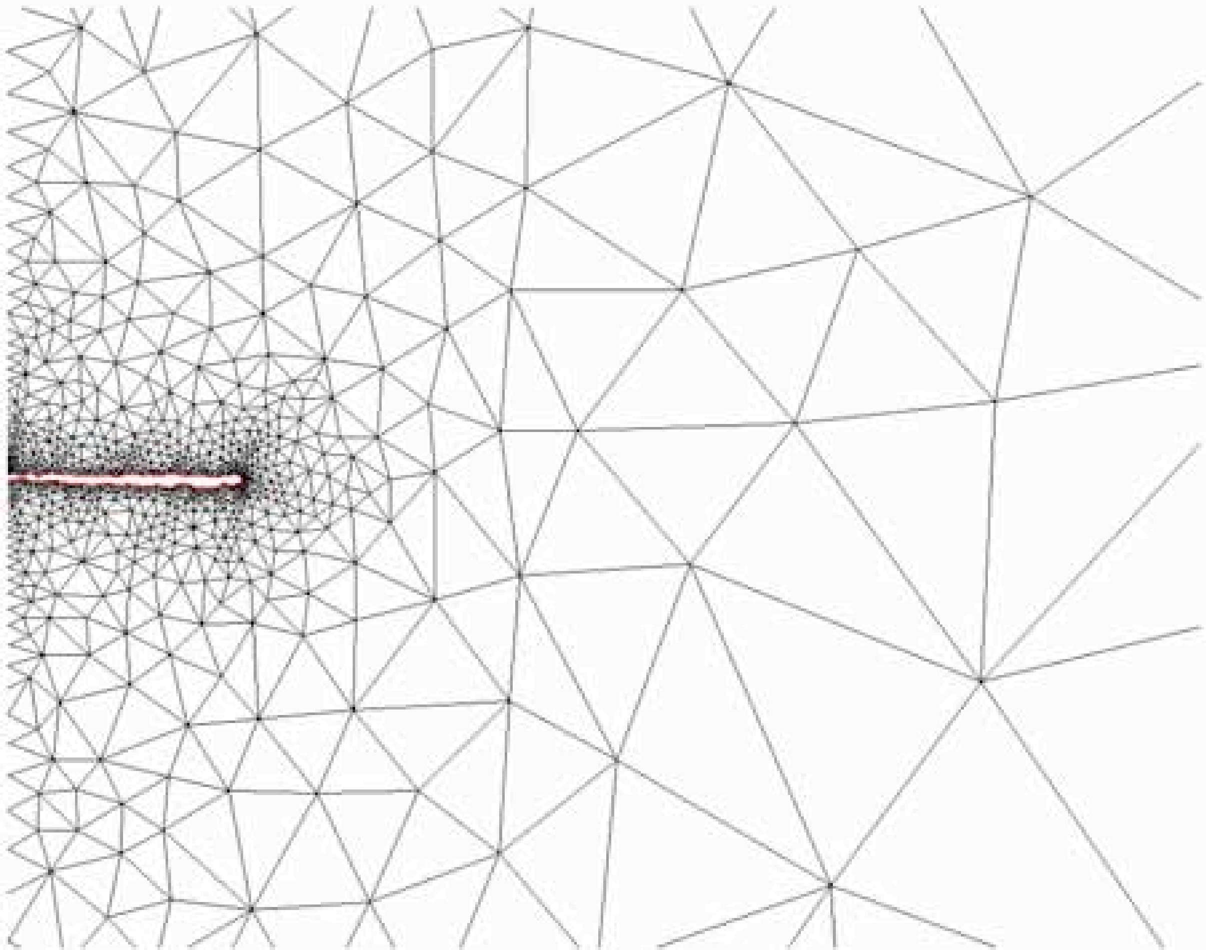

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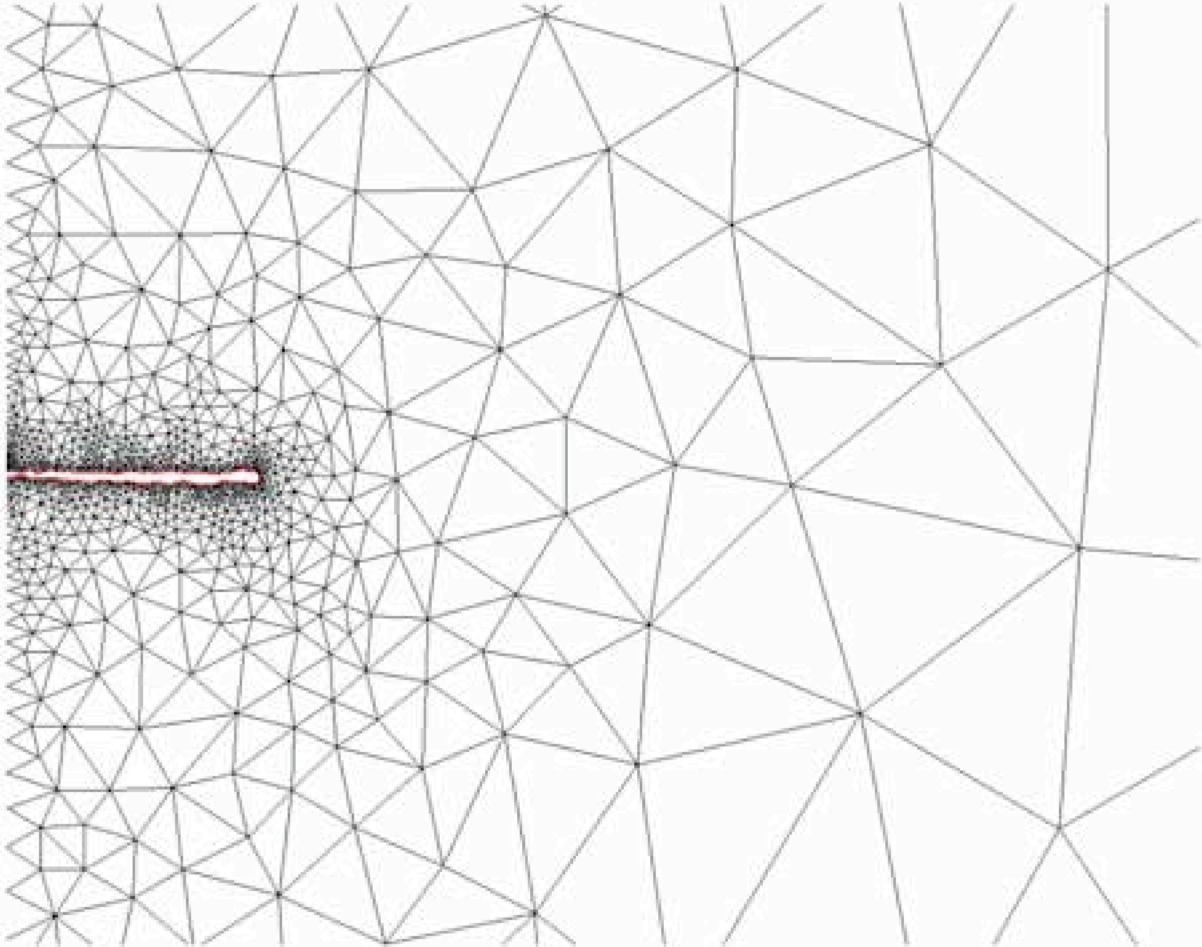

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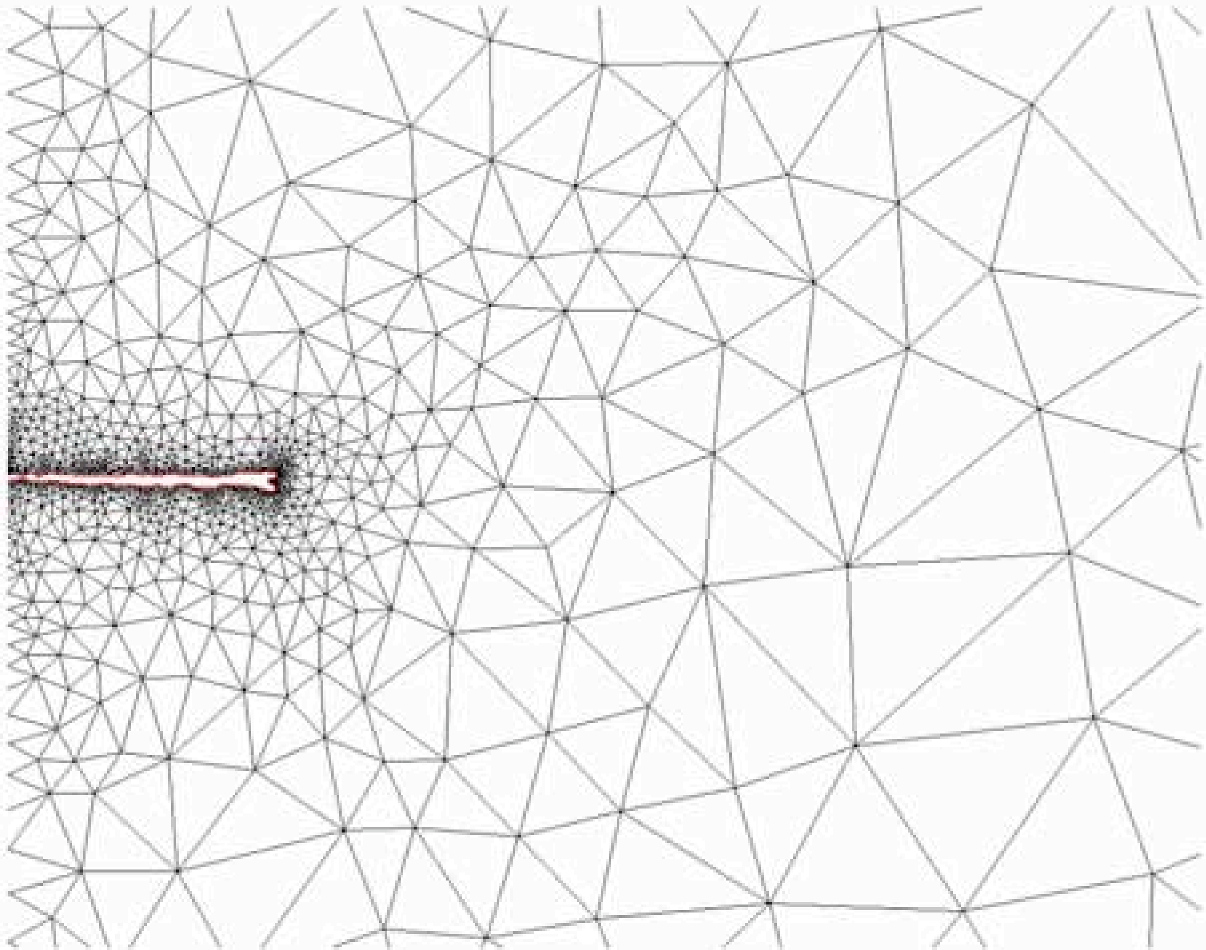

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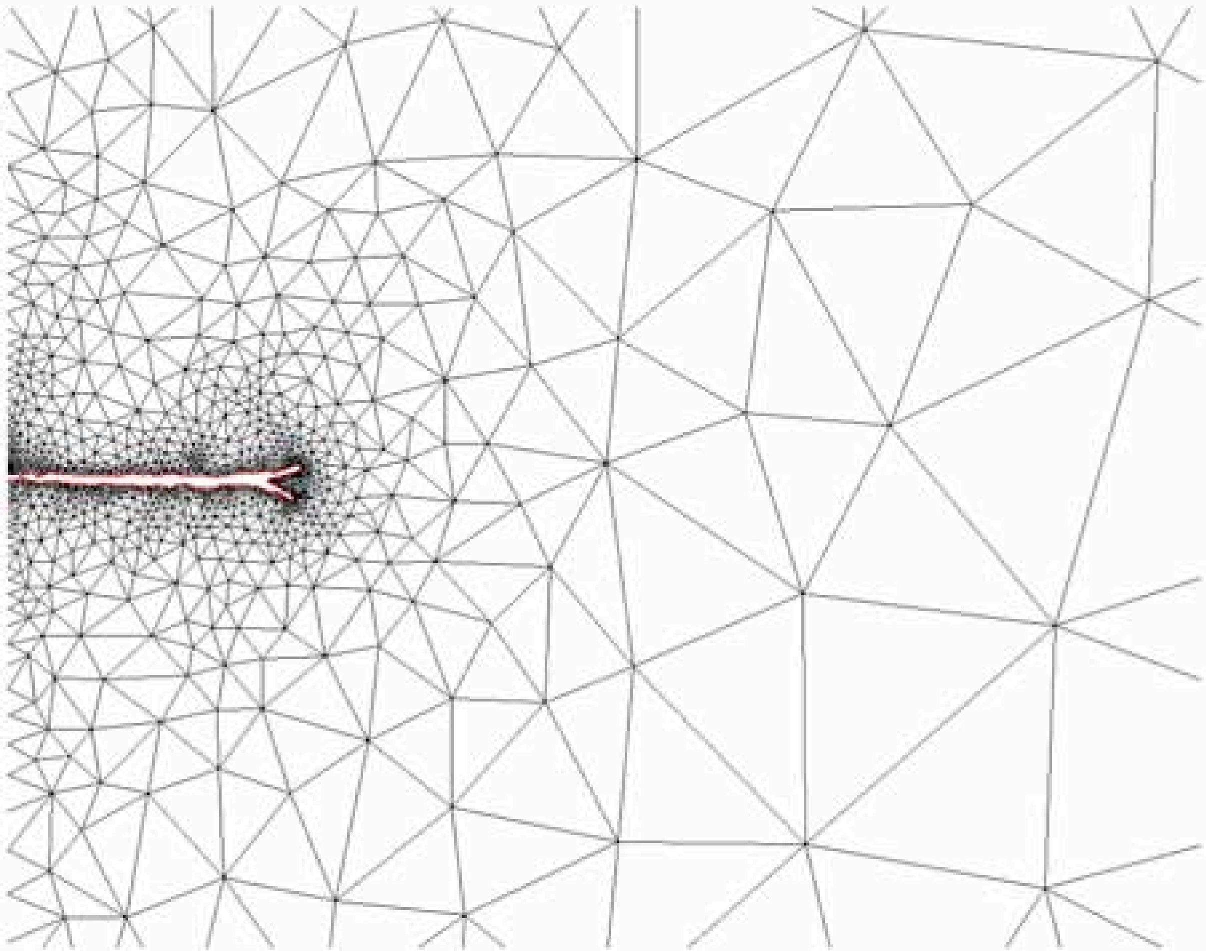

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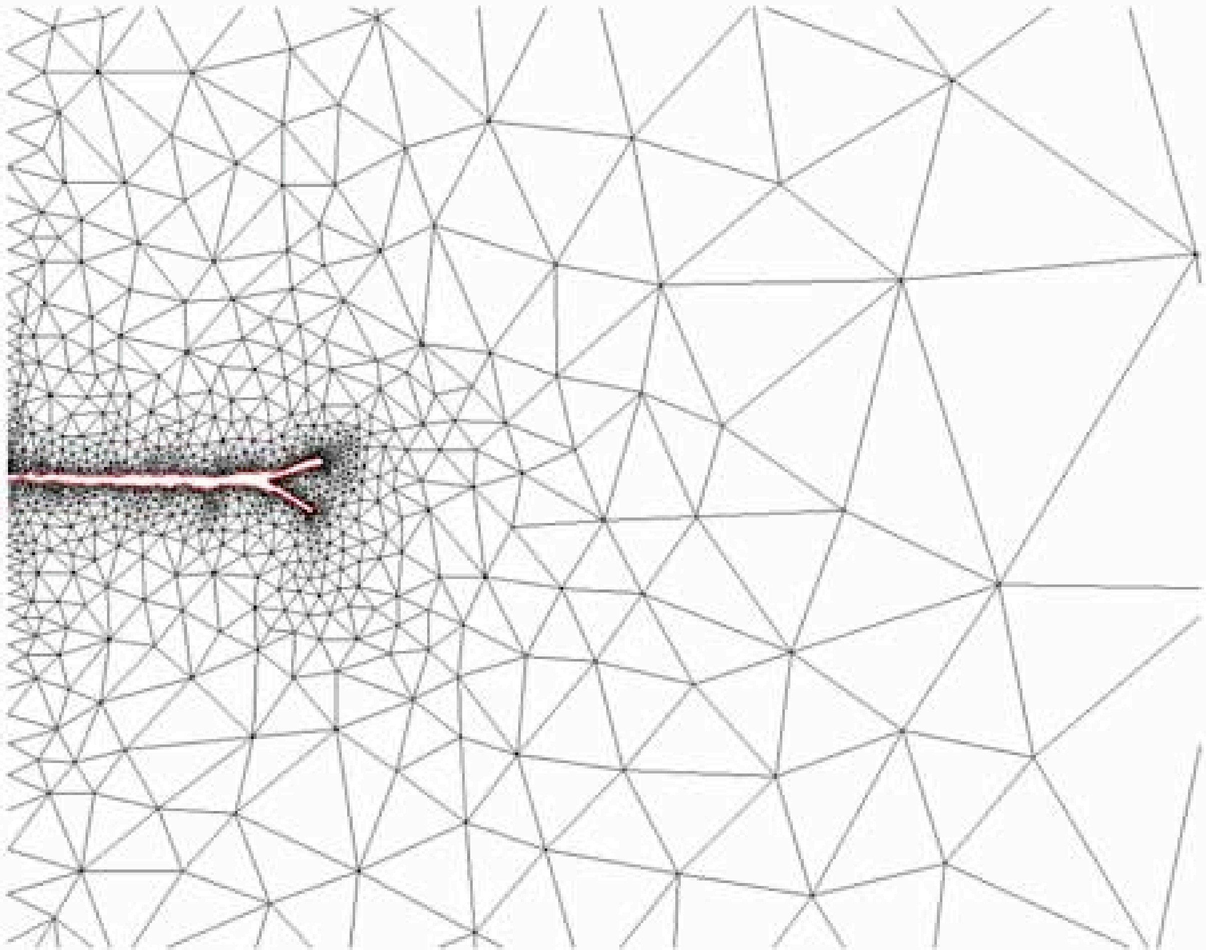

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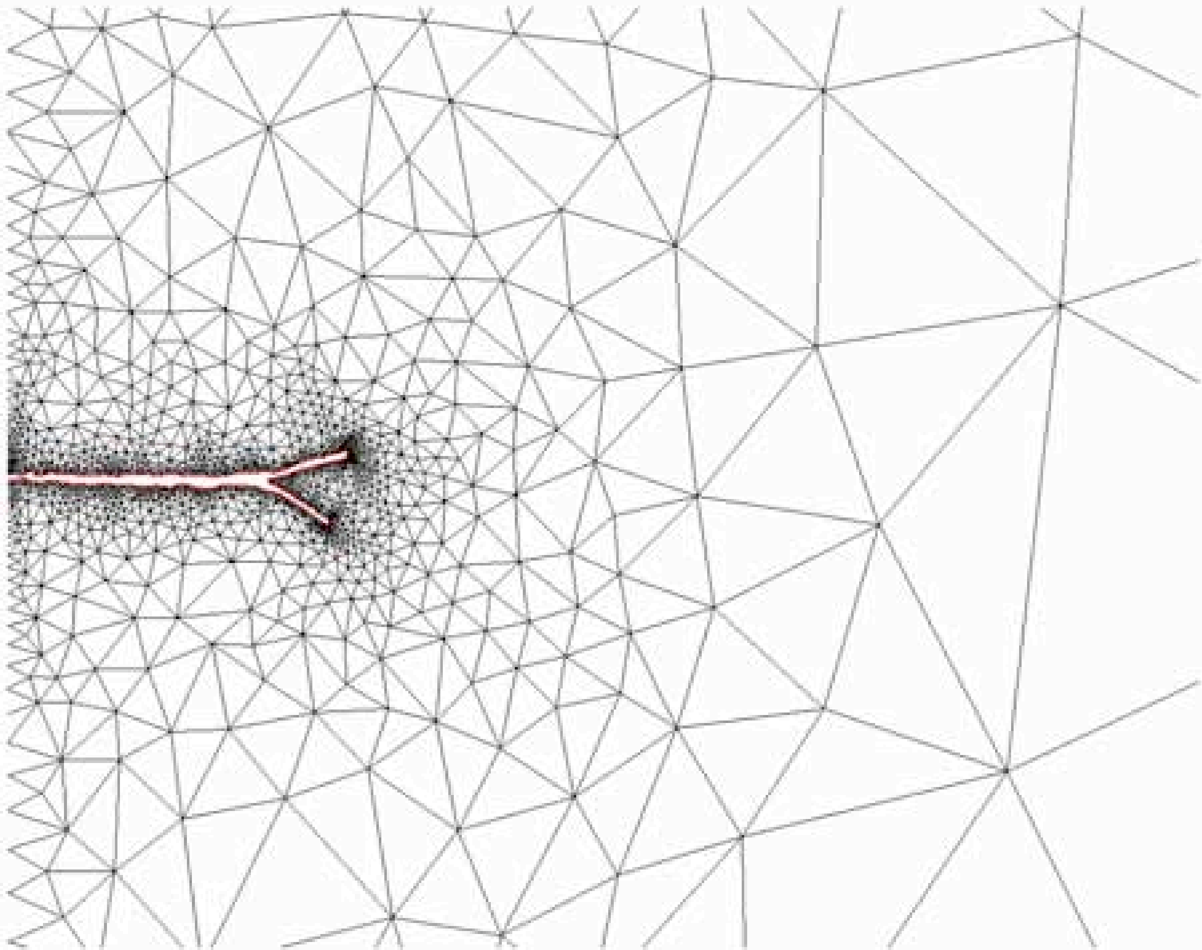

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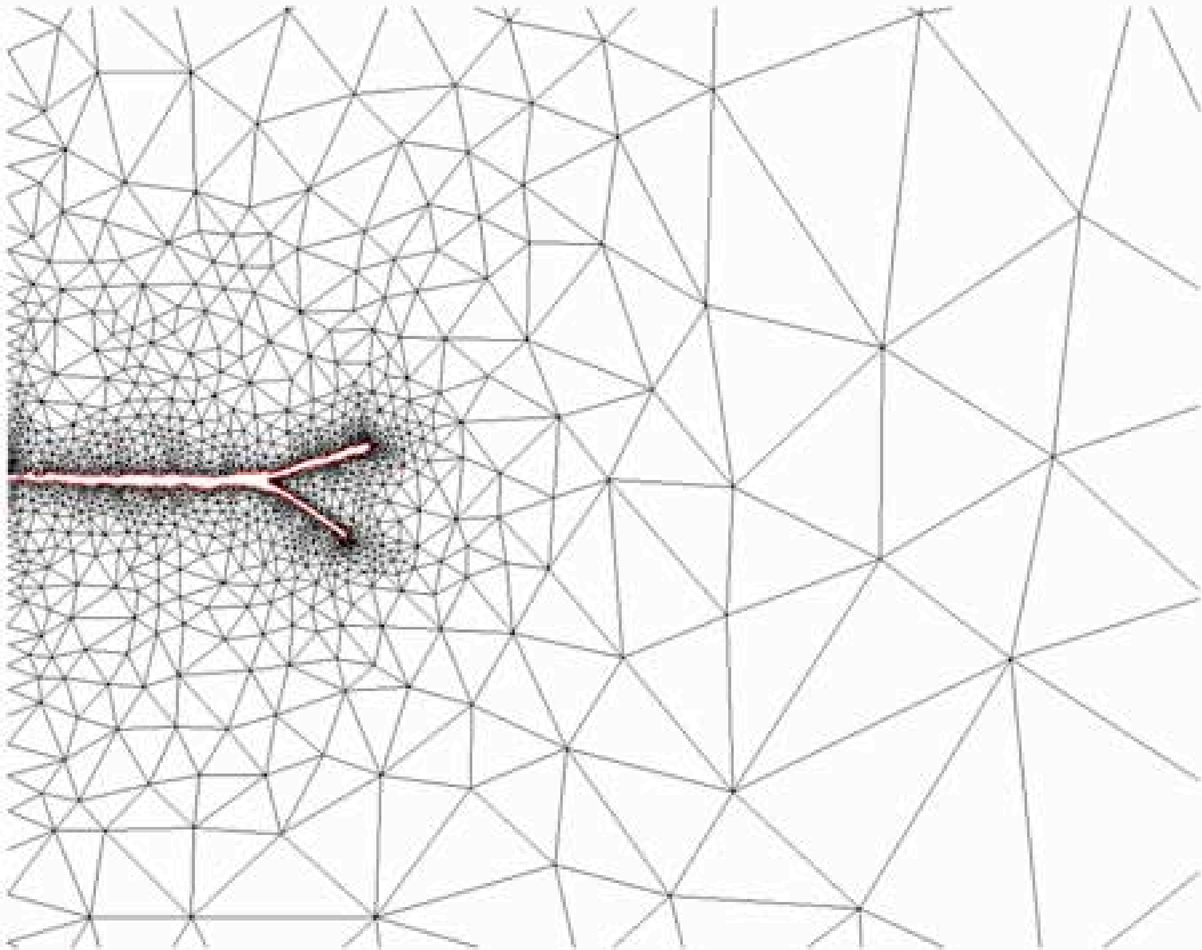

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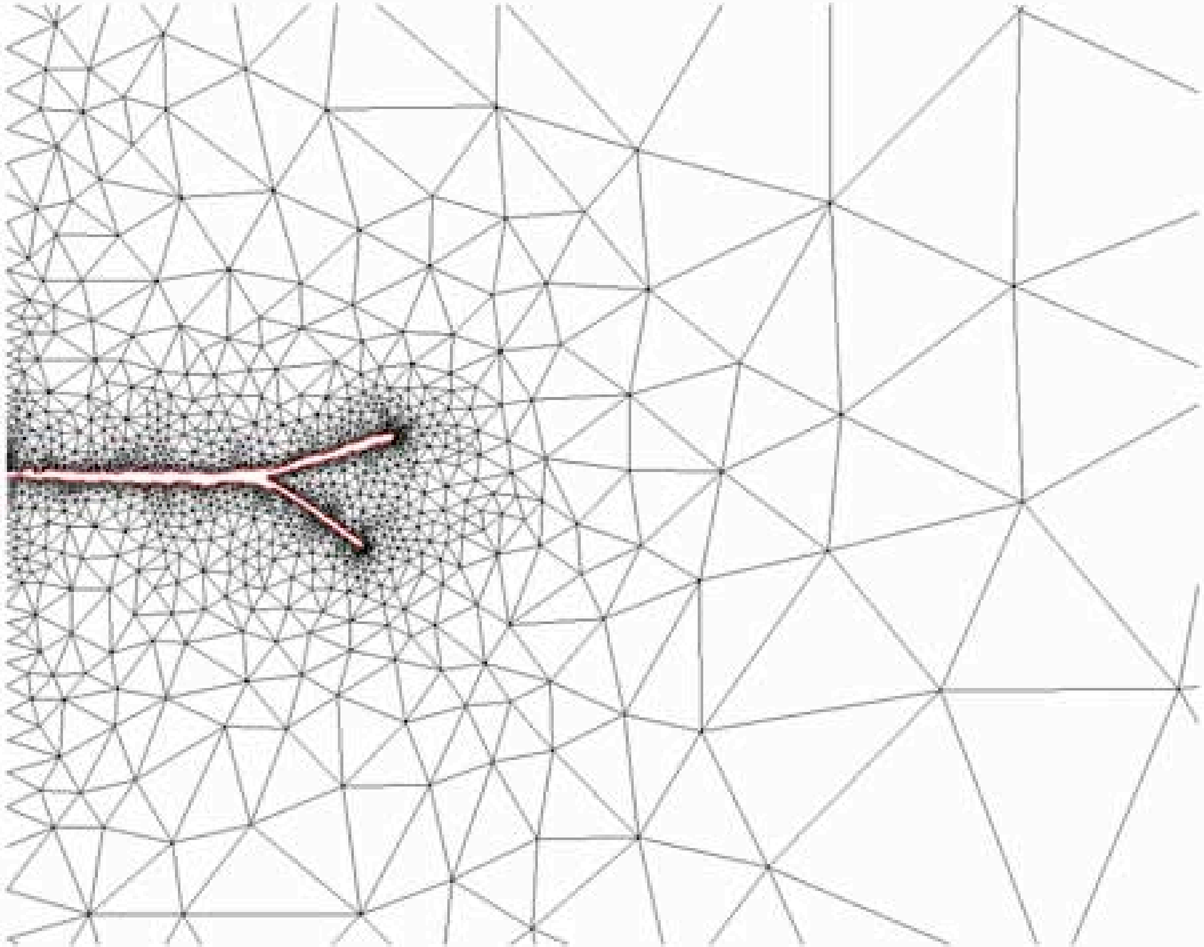

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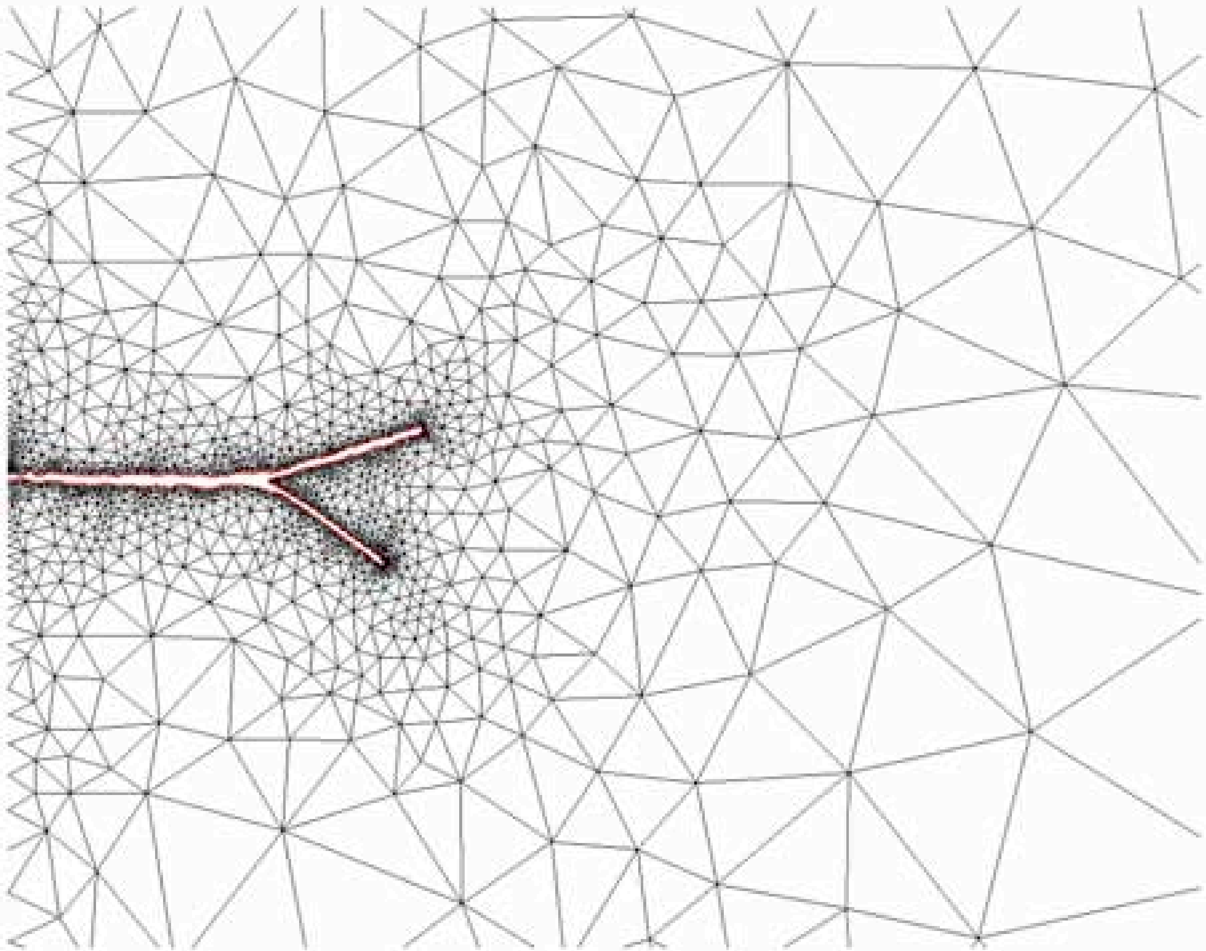

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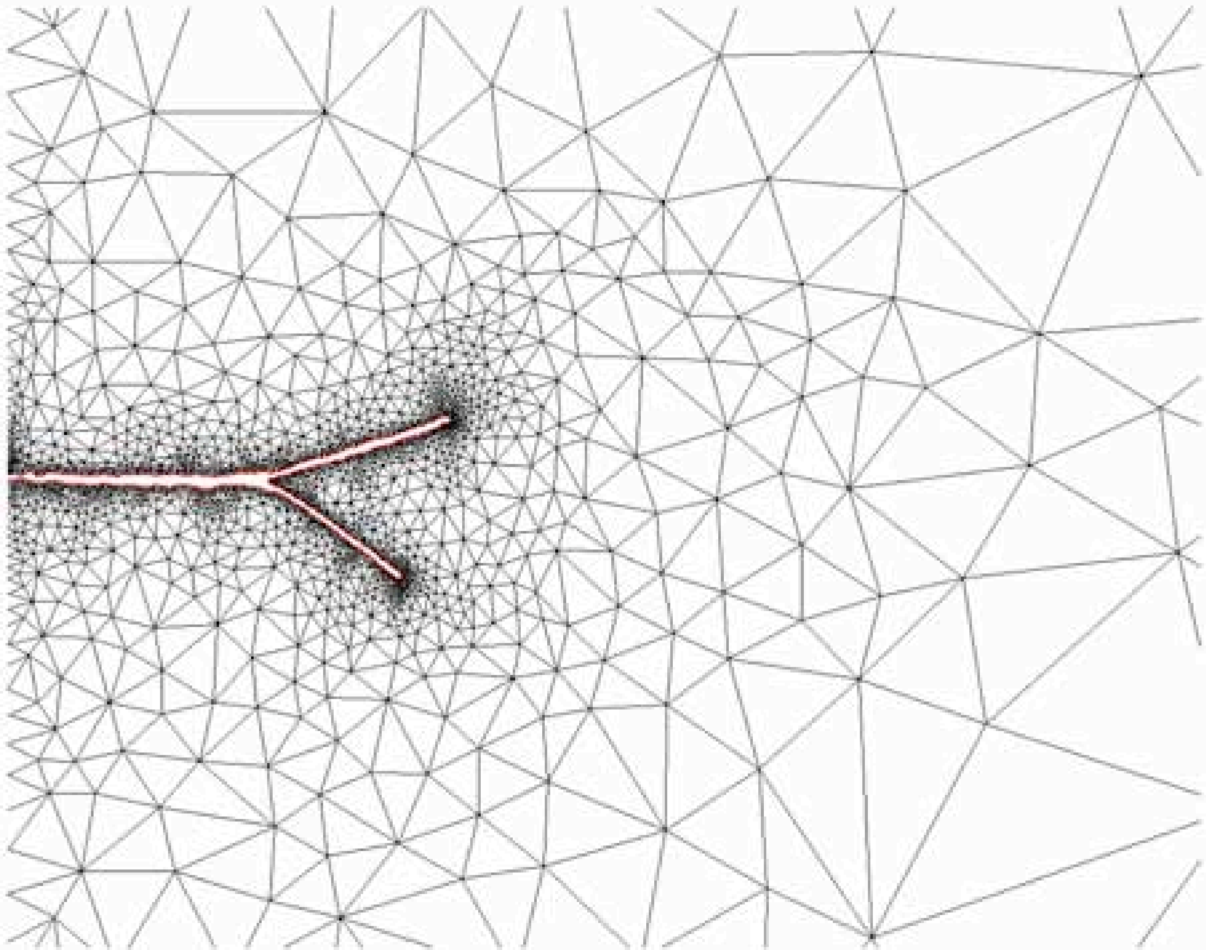

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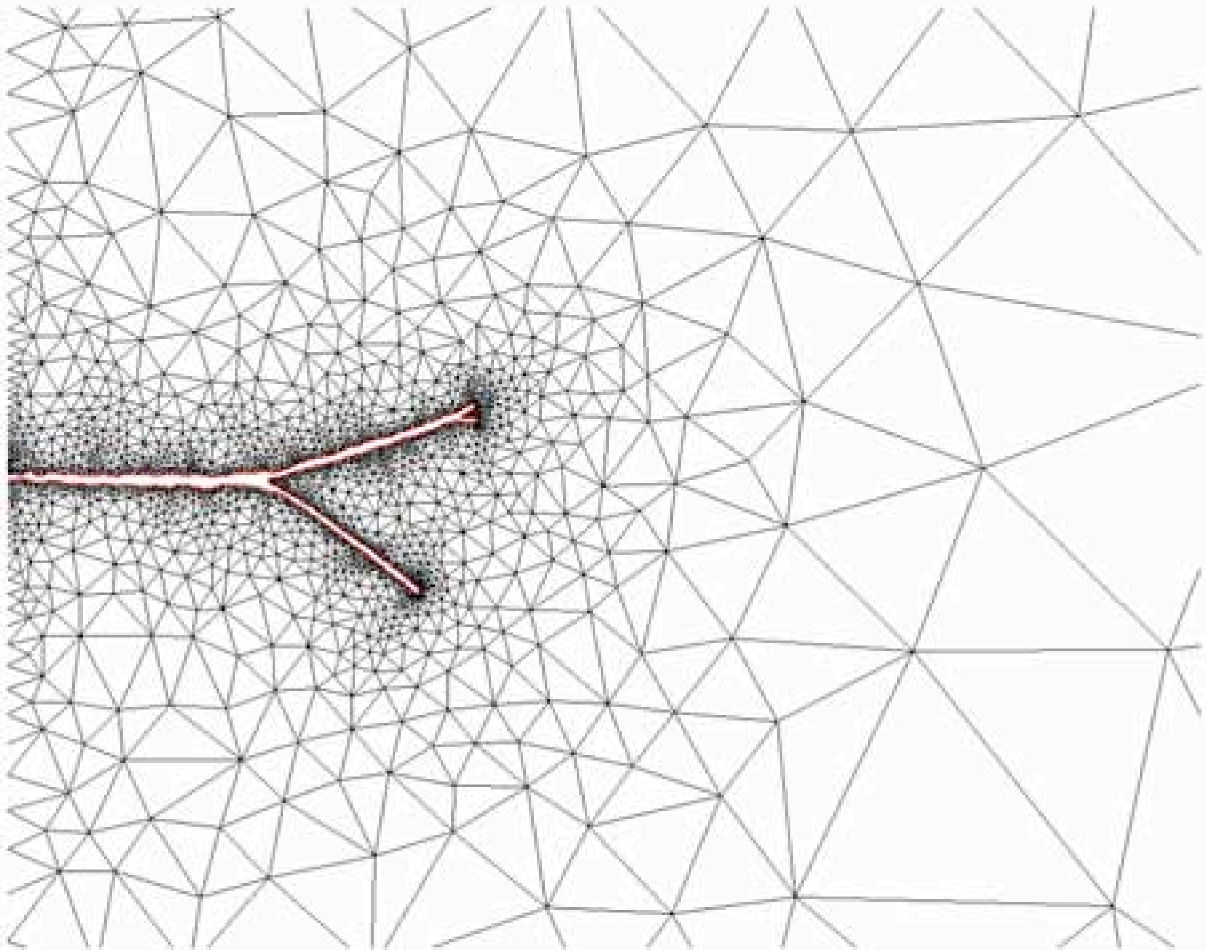
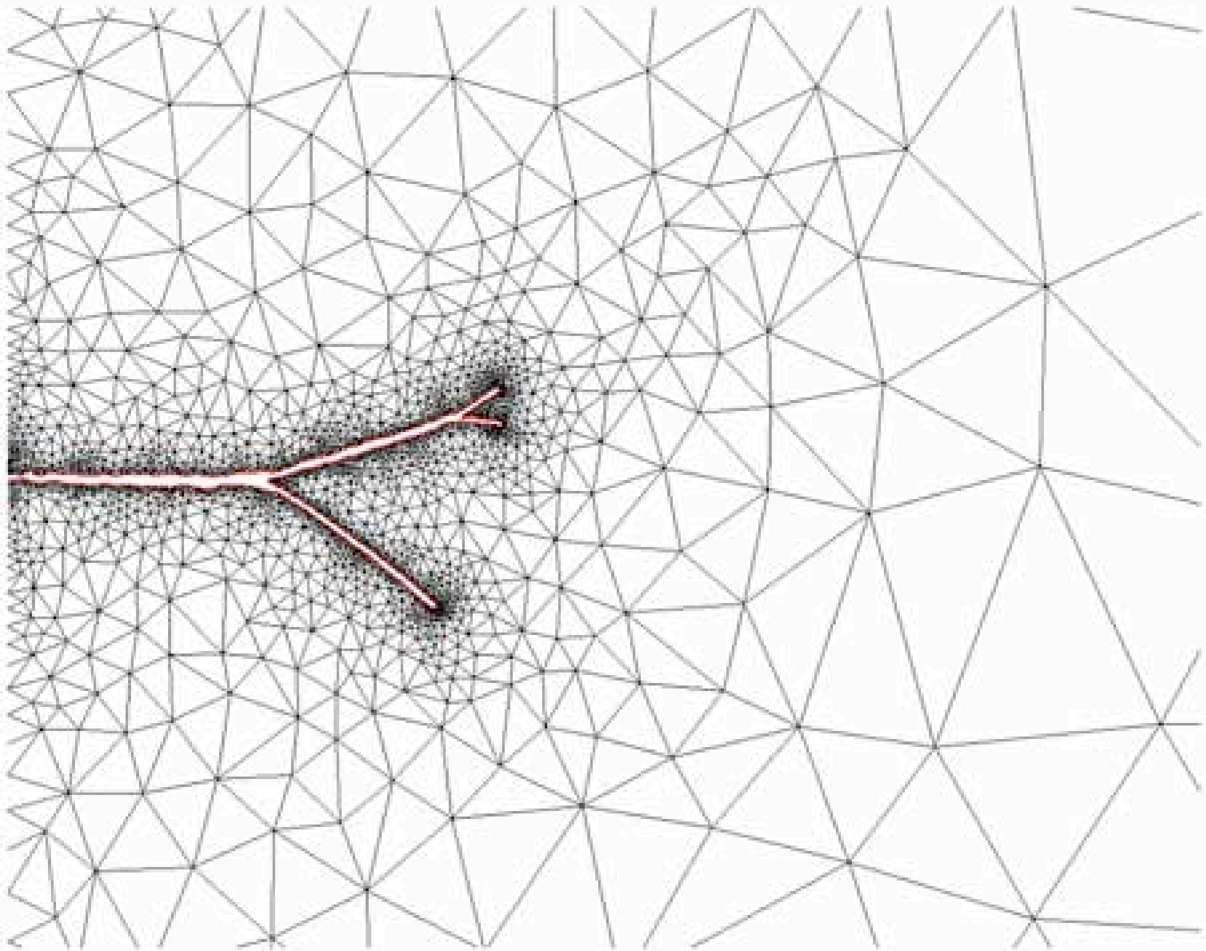


Branching



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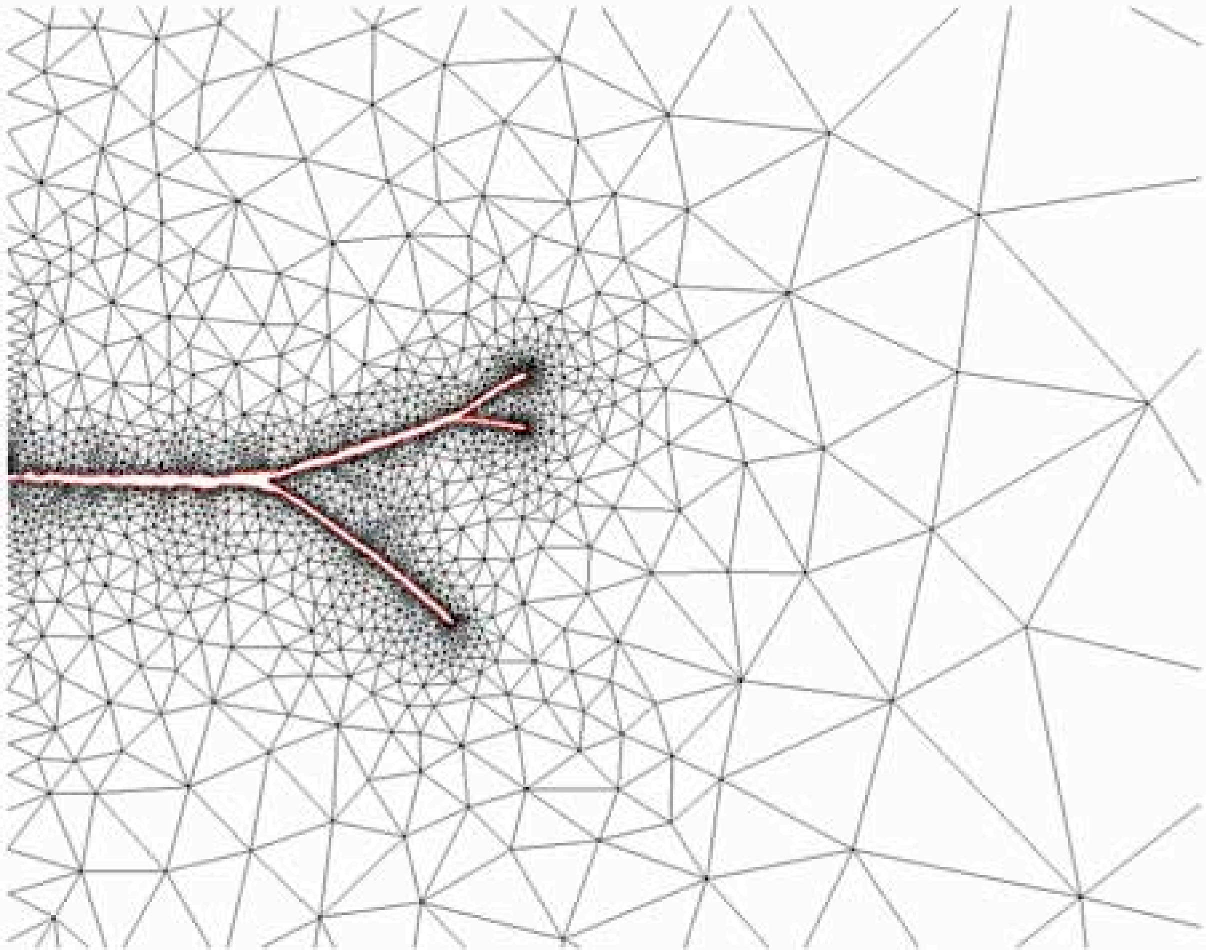

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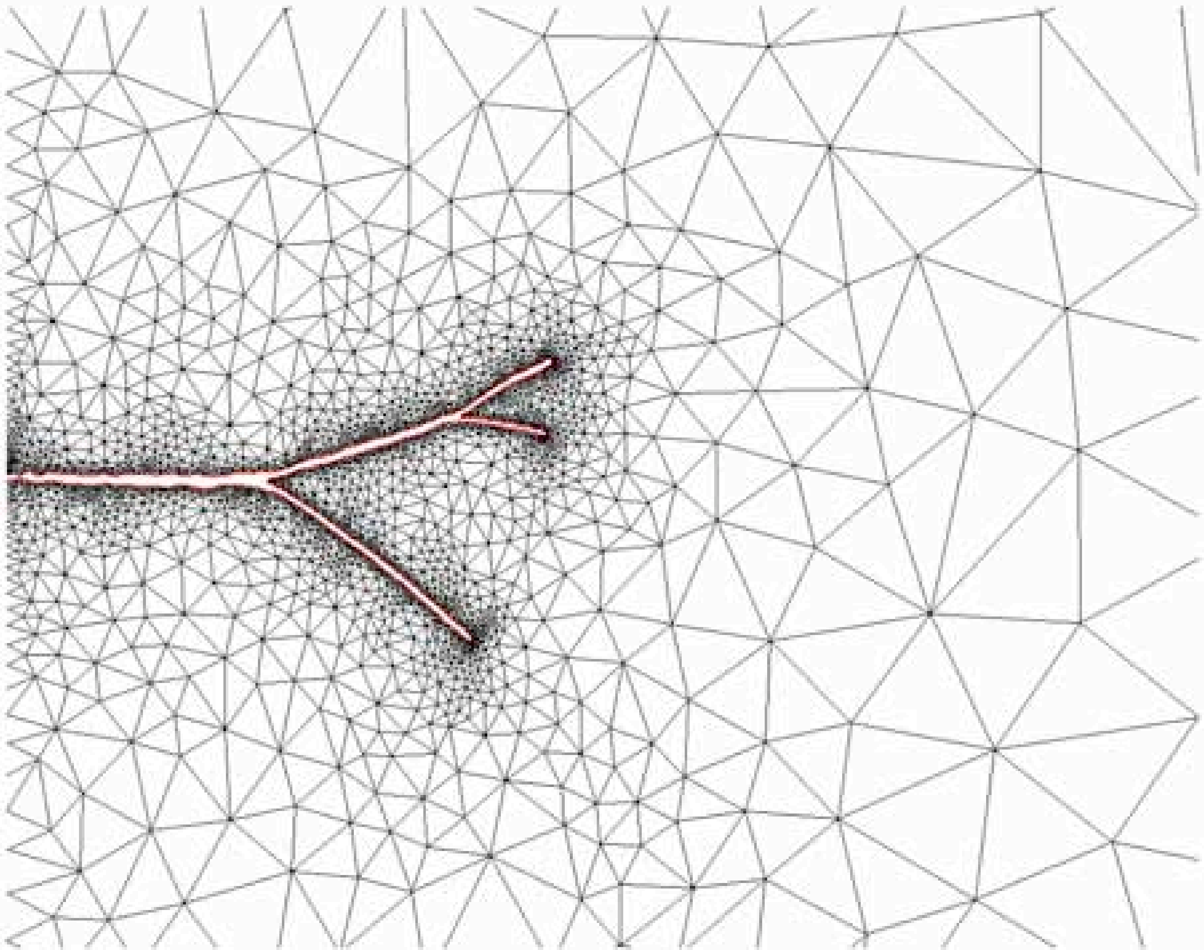

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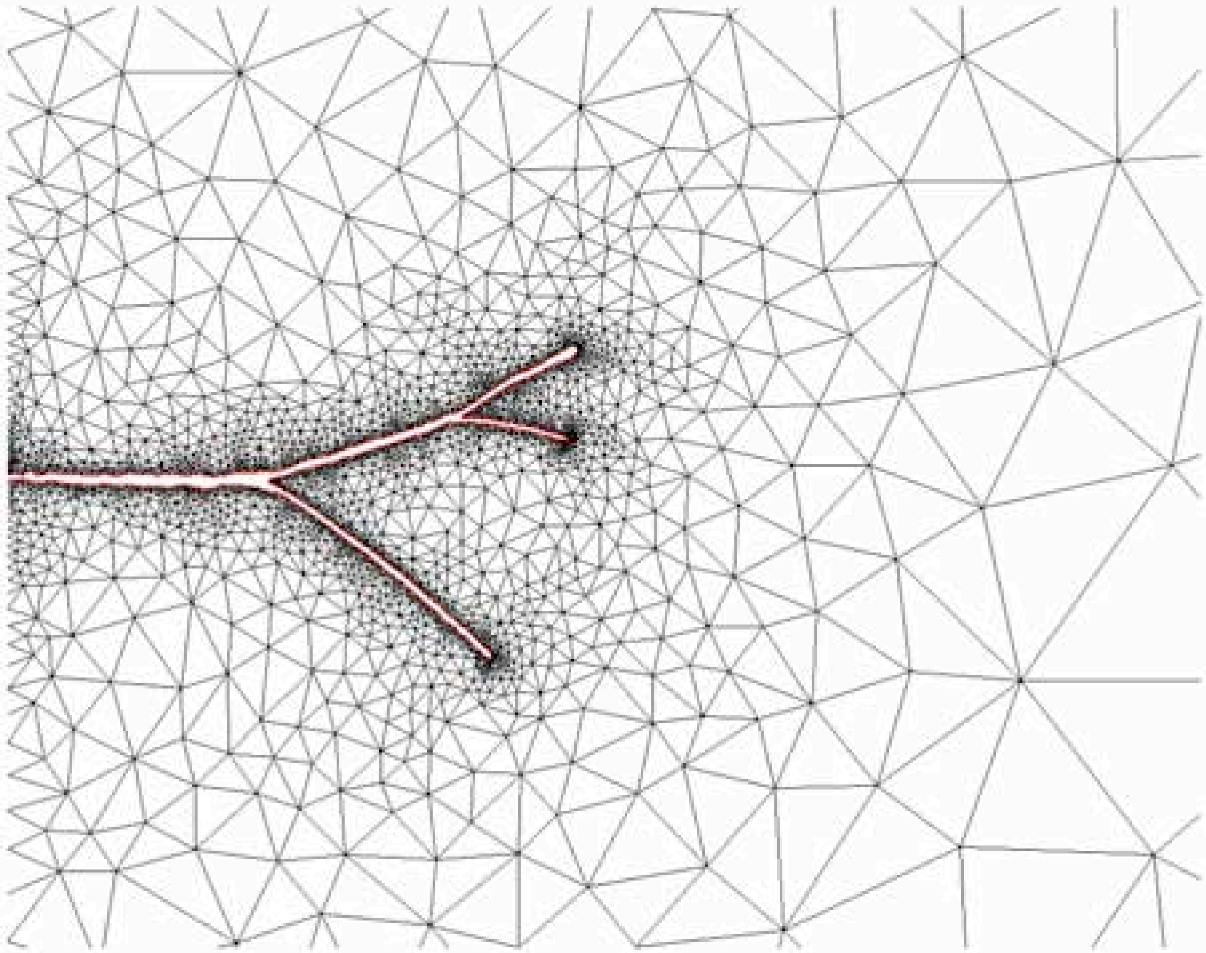

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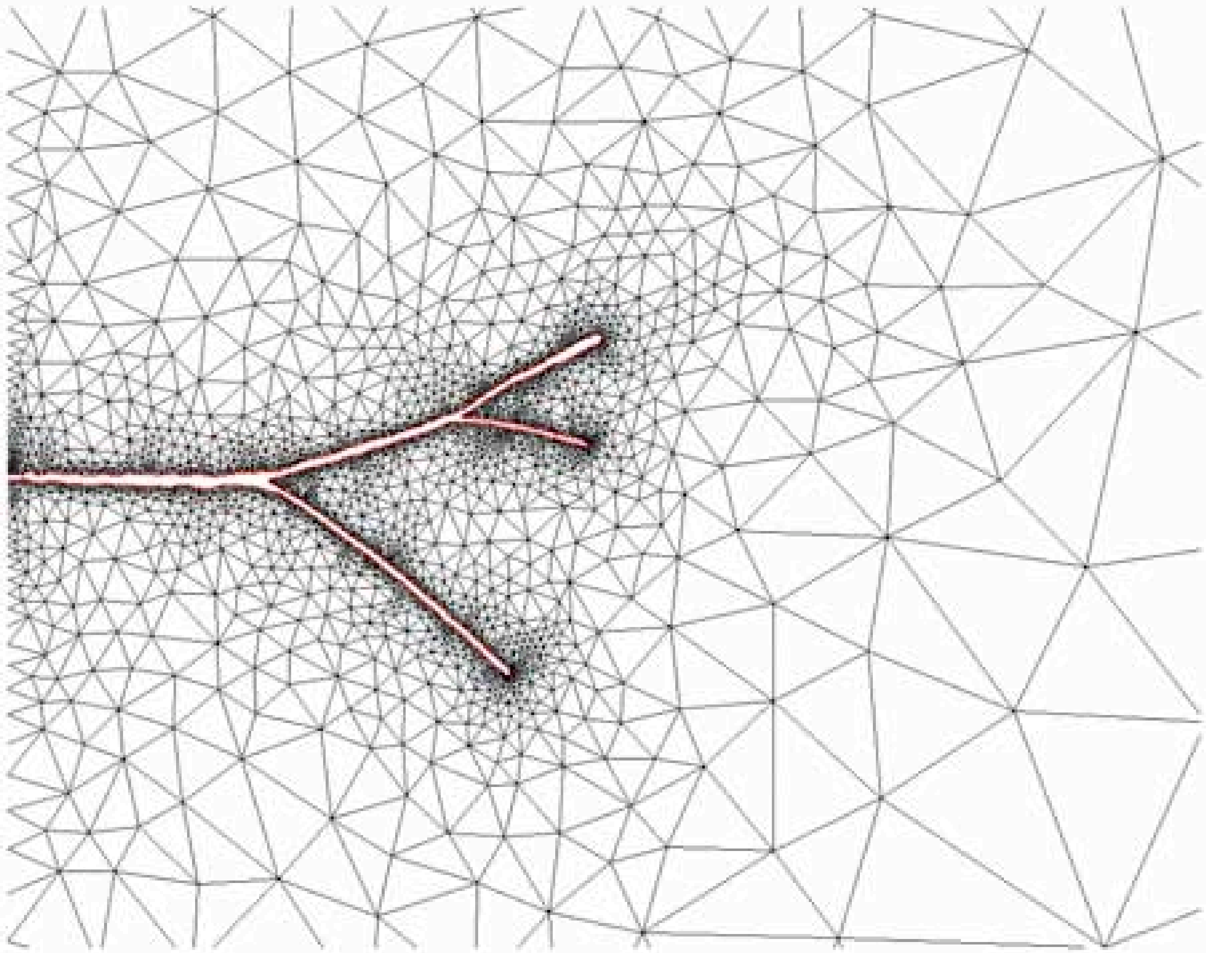

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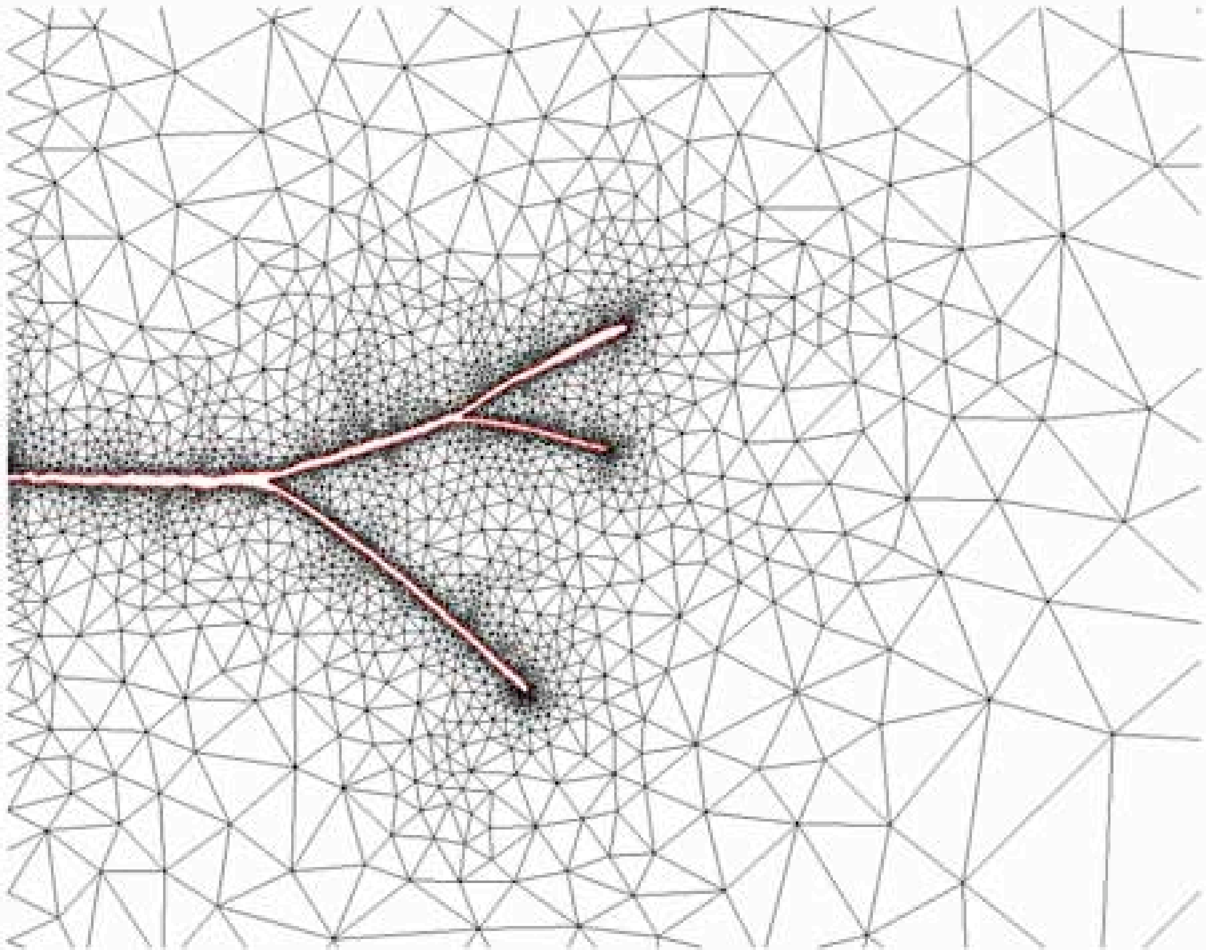

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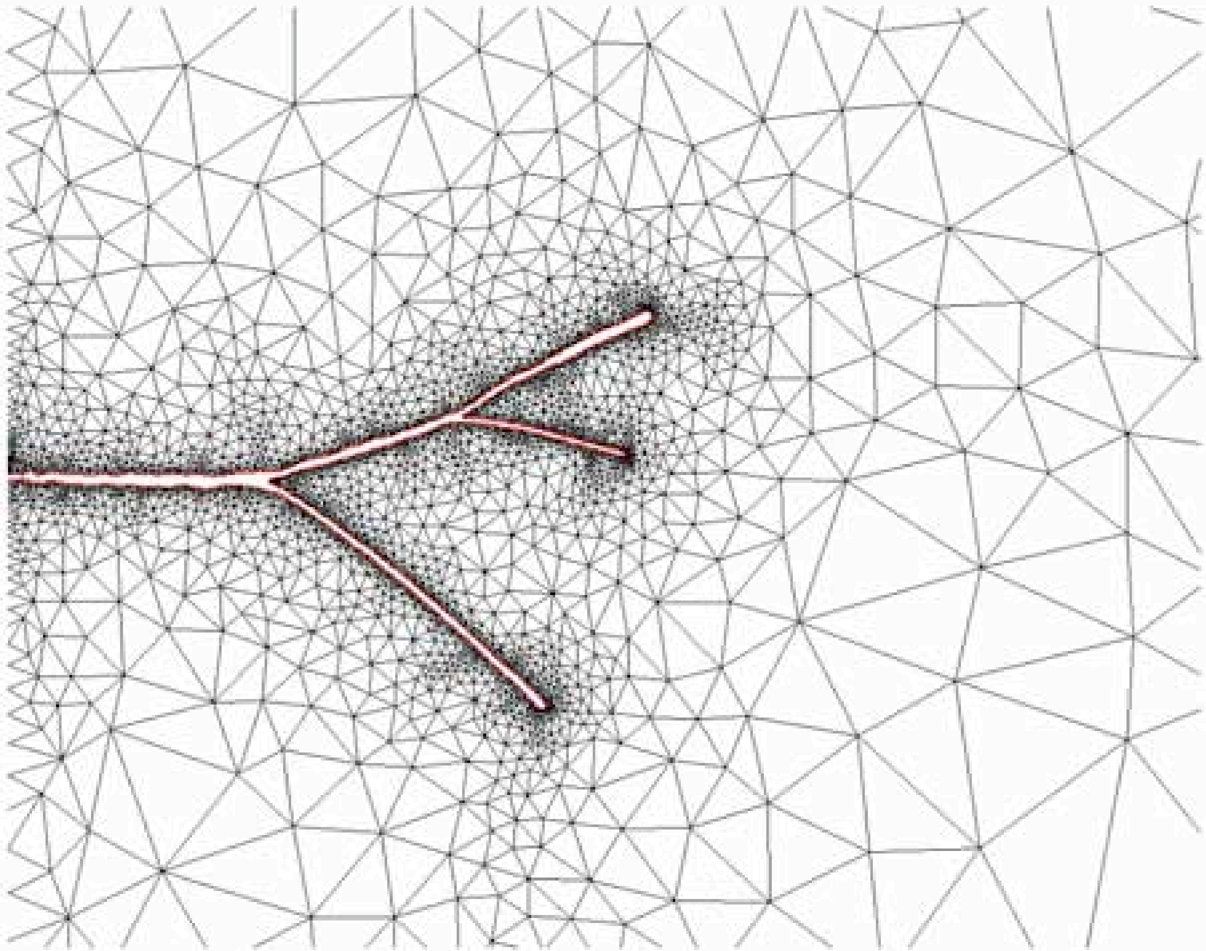

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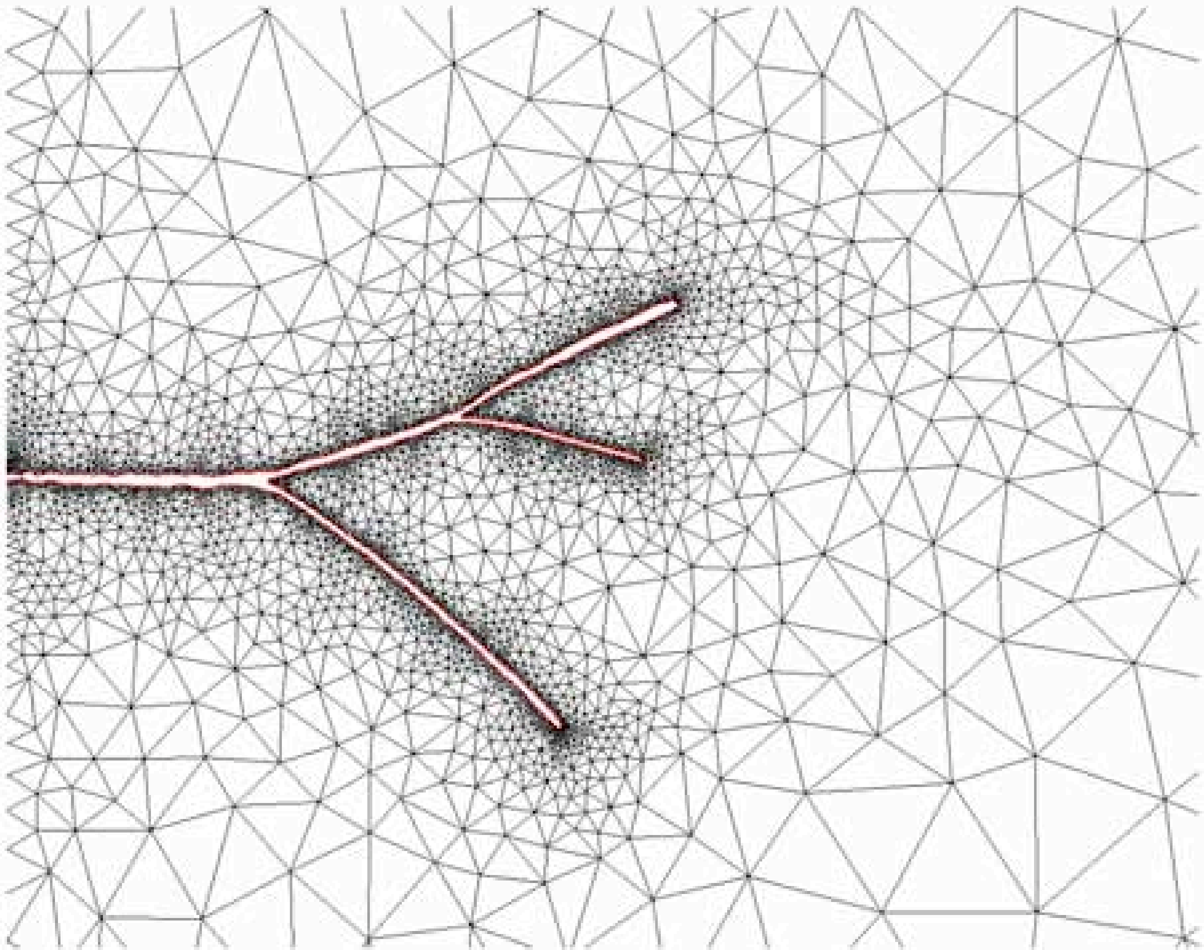

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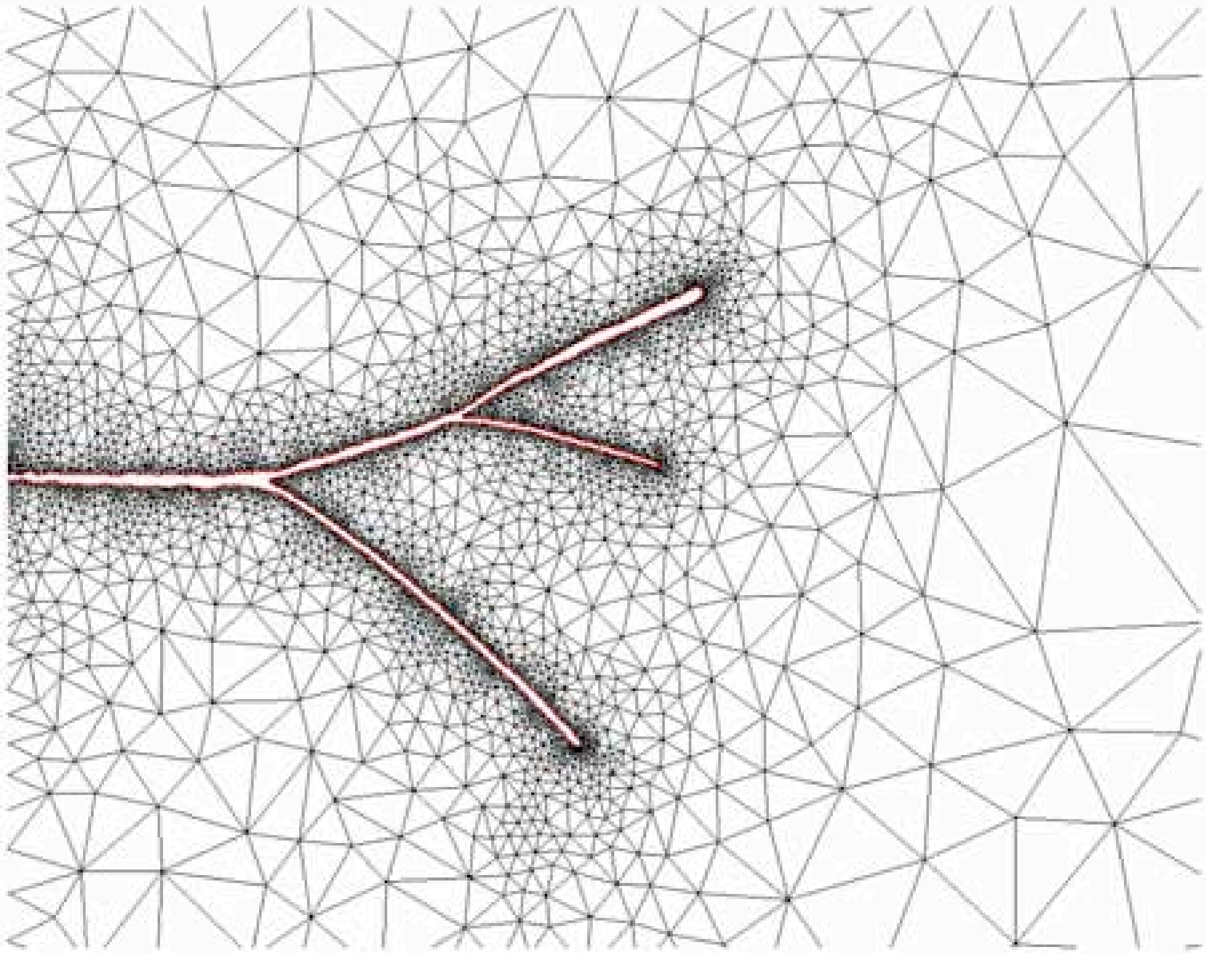

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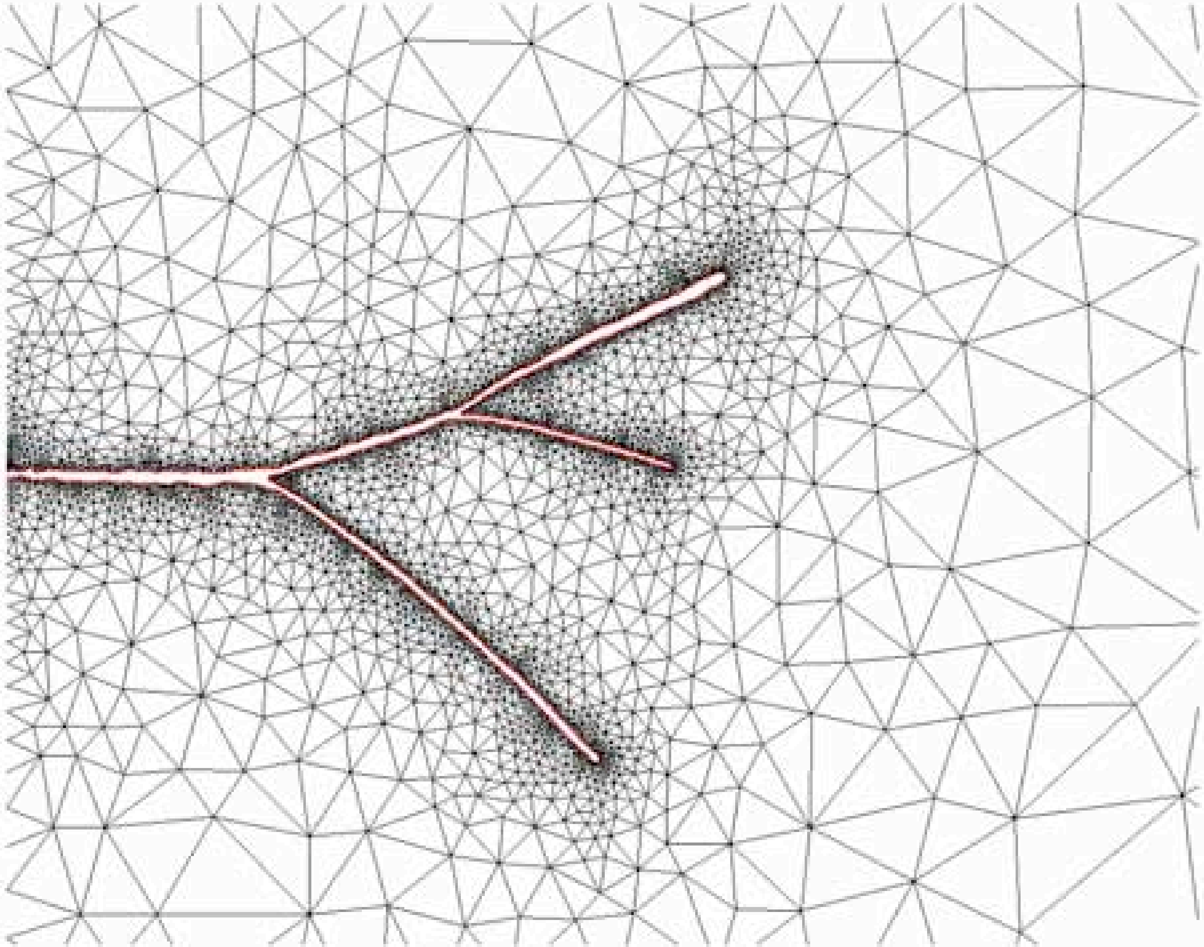

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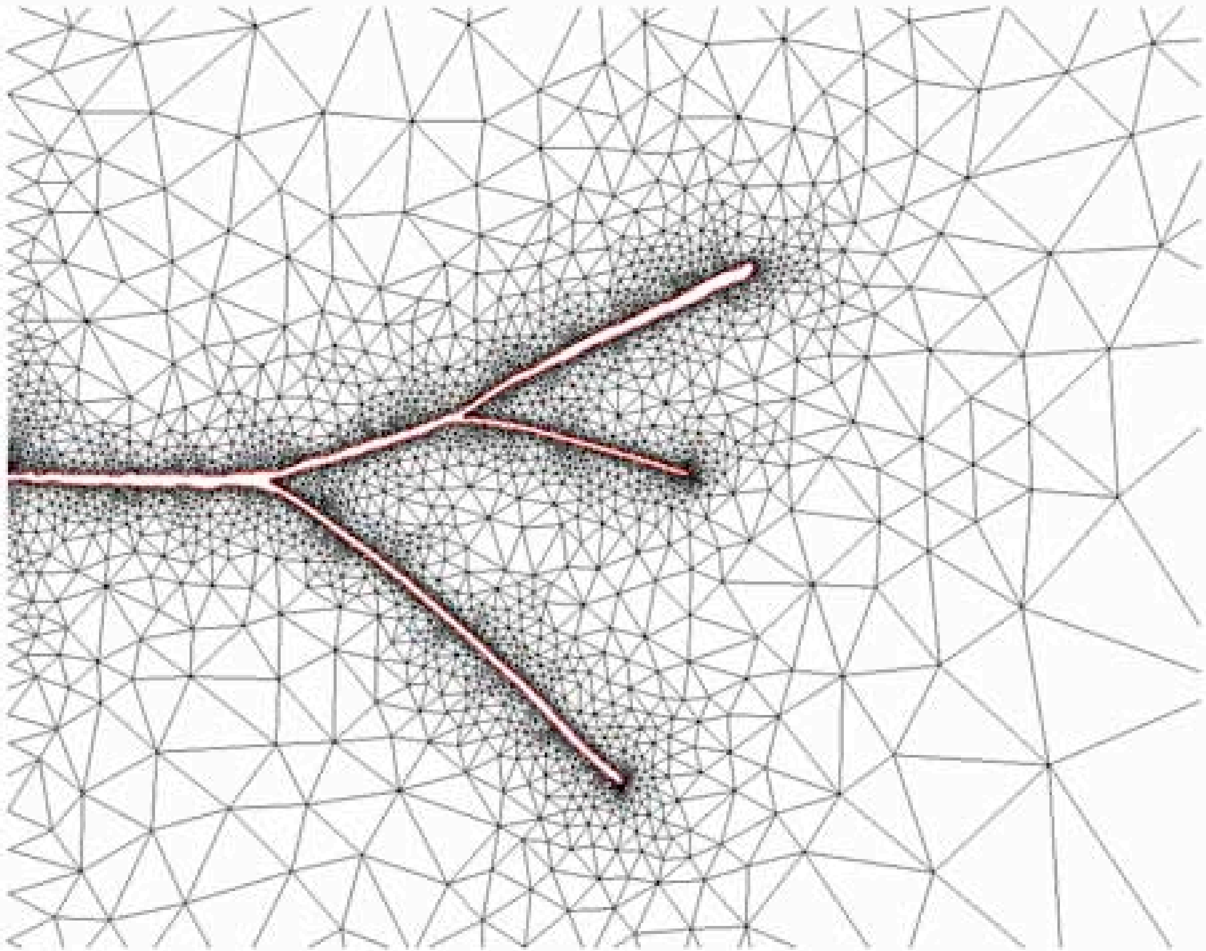

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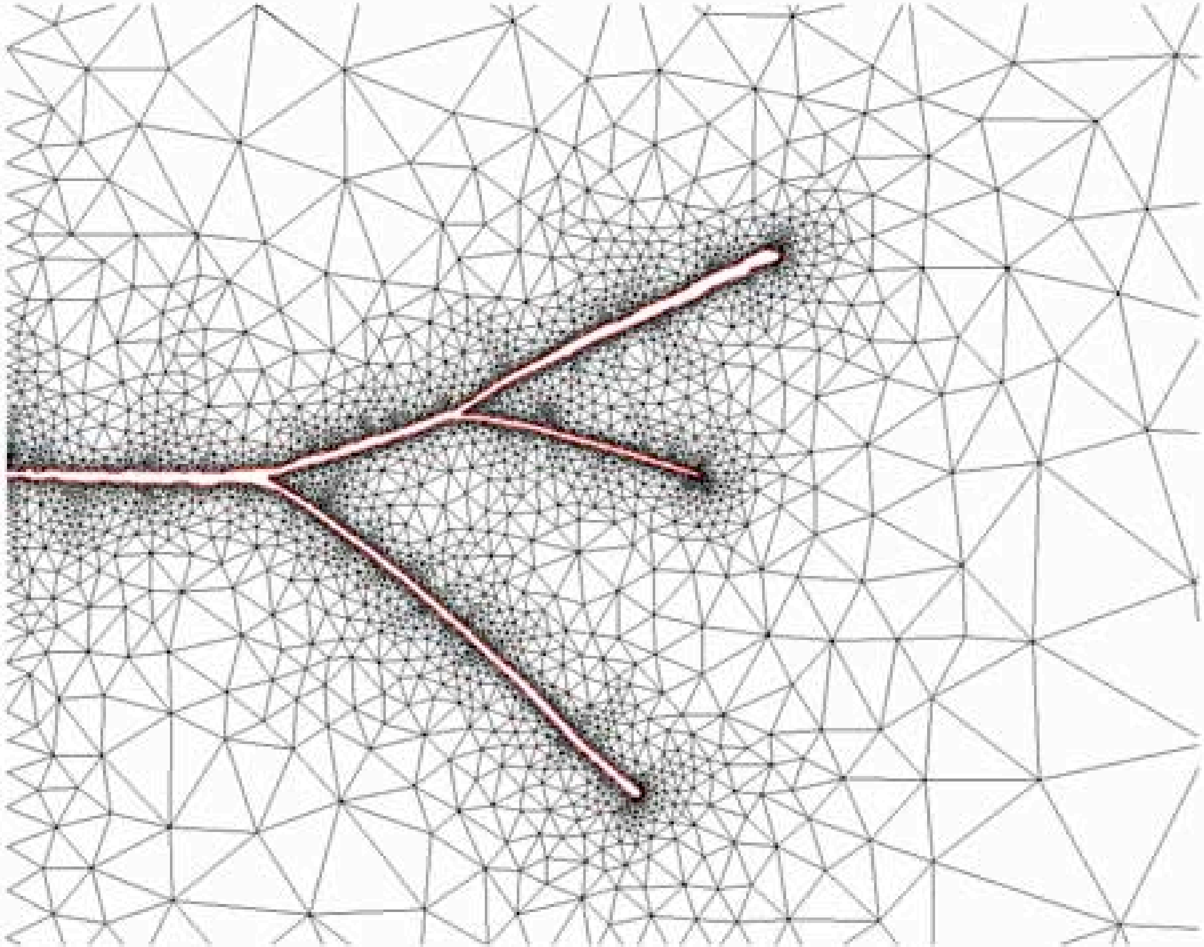

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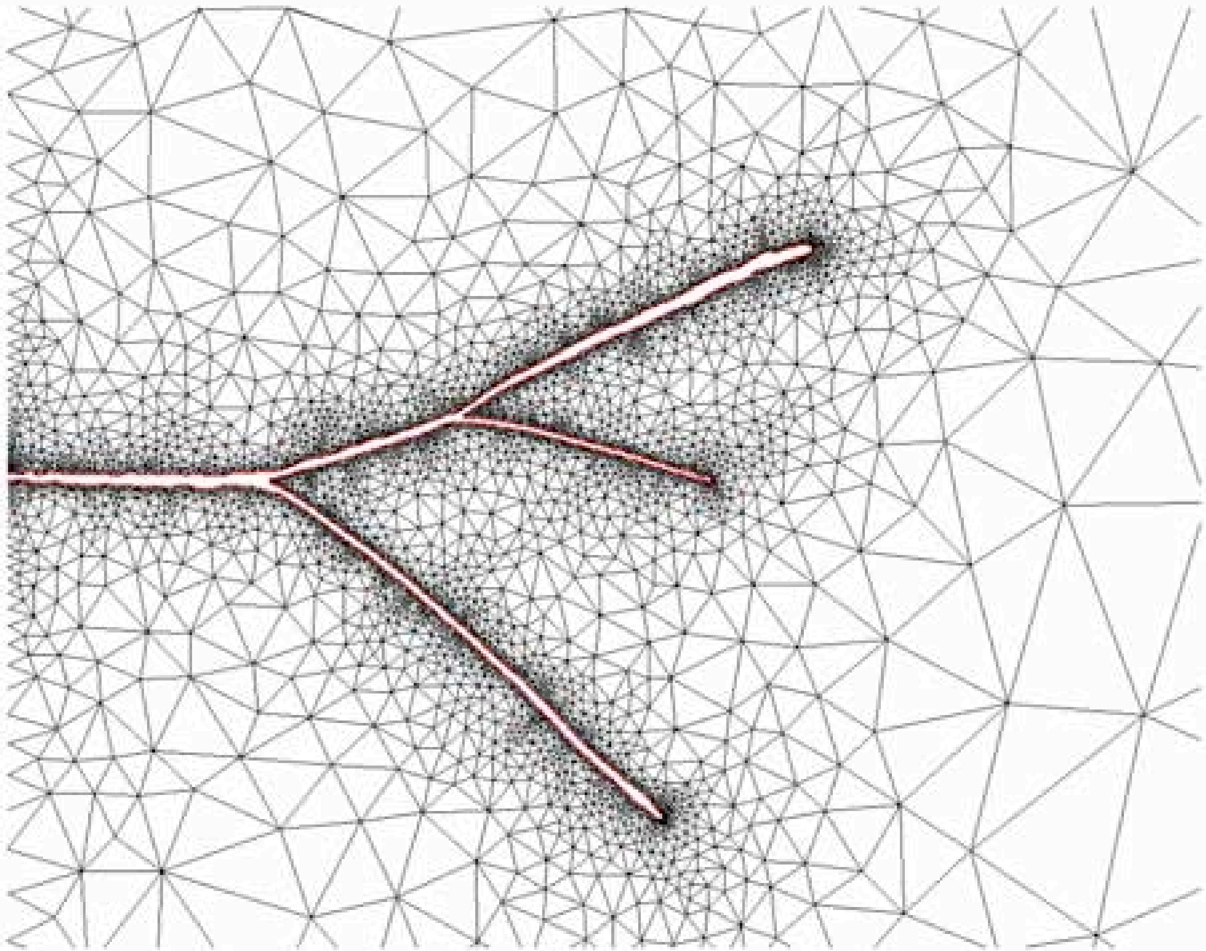

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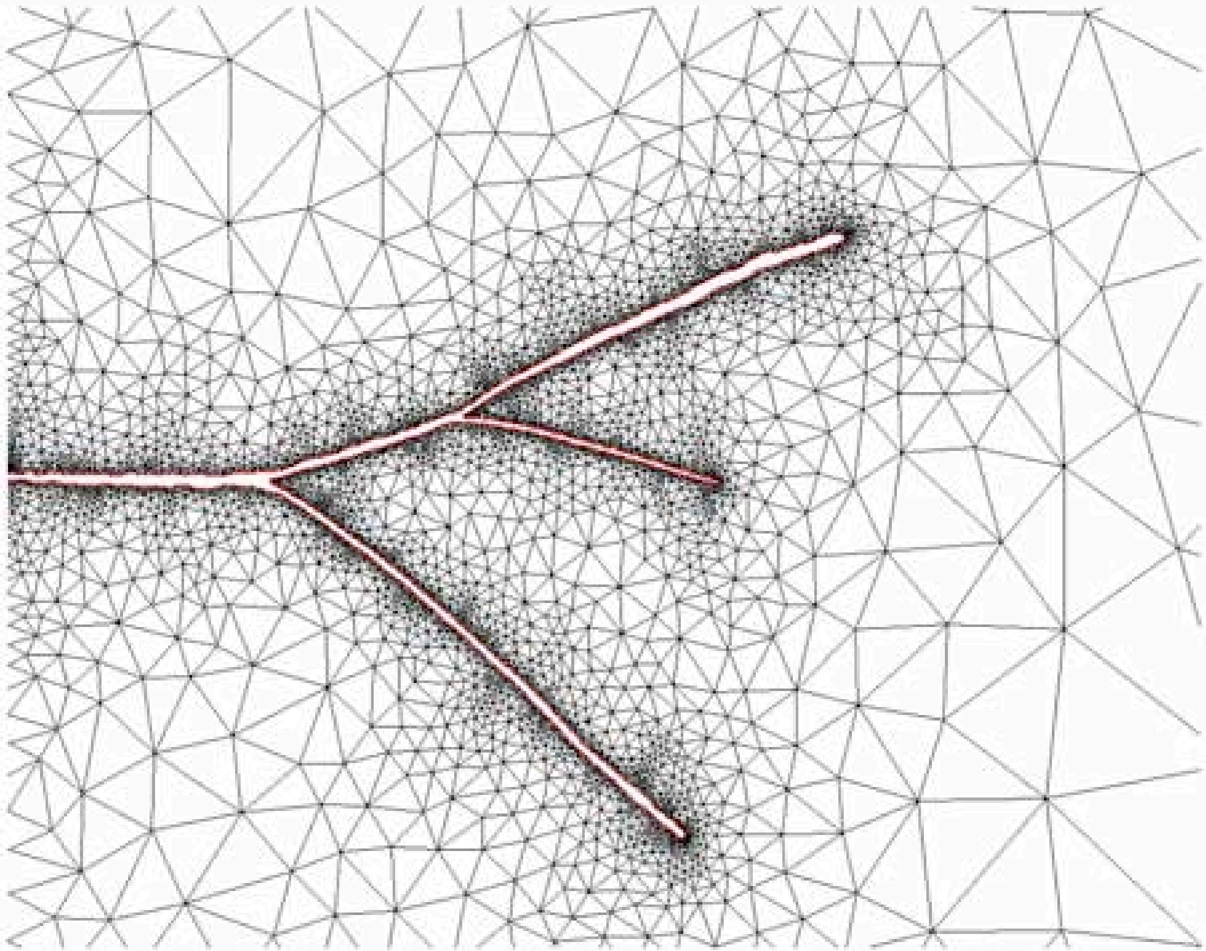

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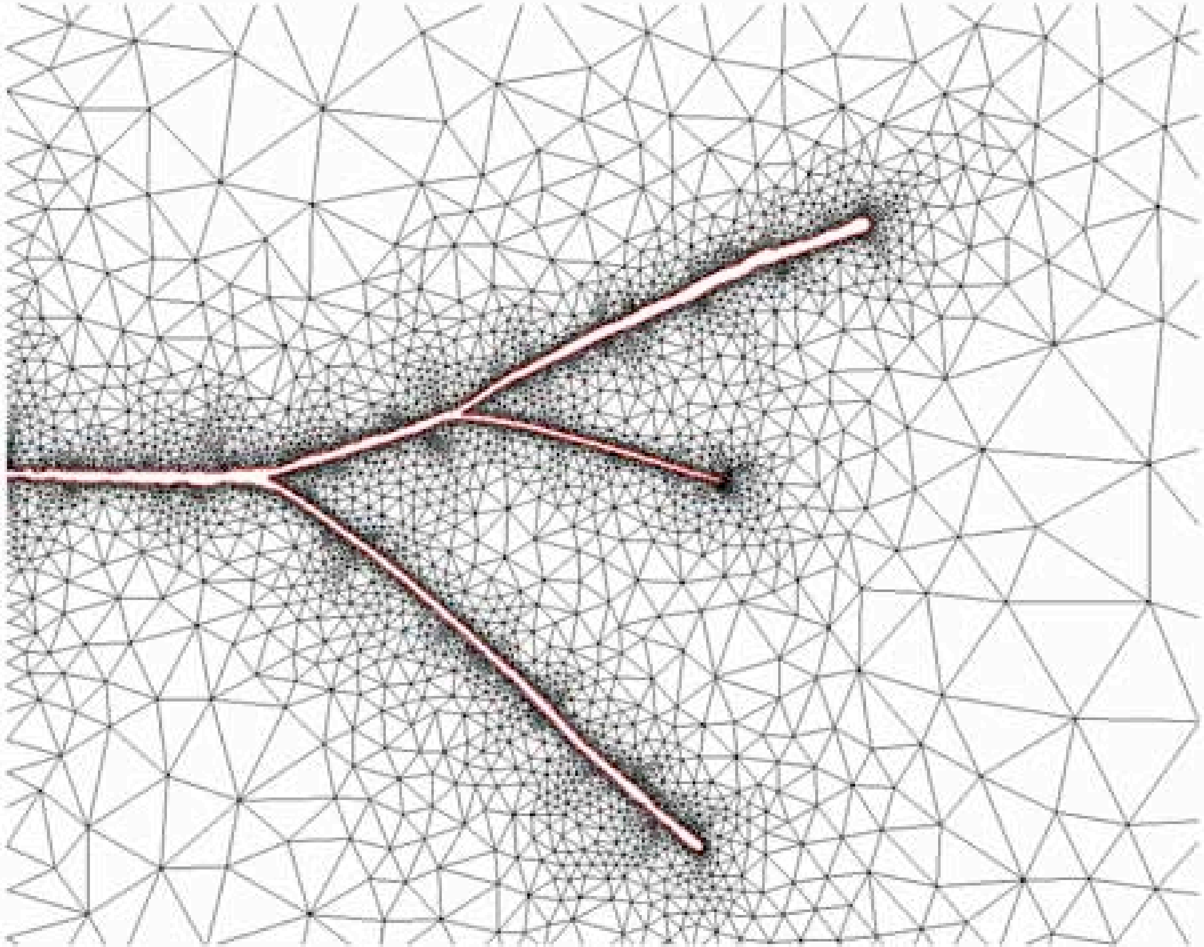

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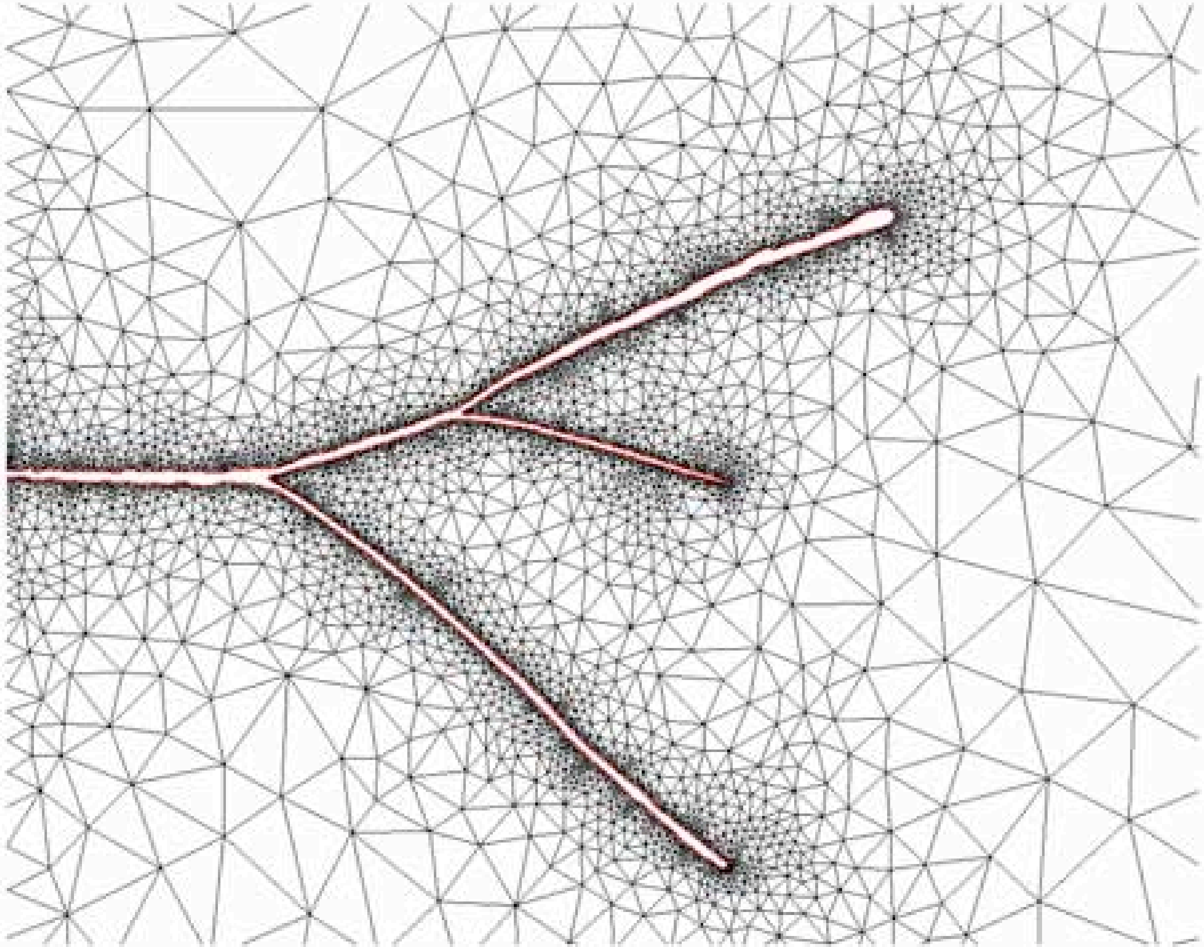

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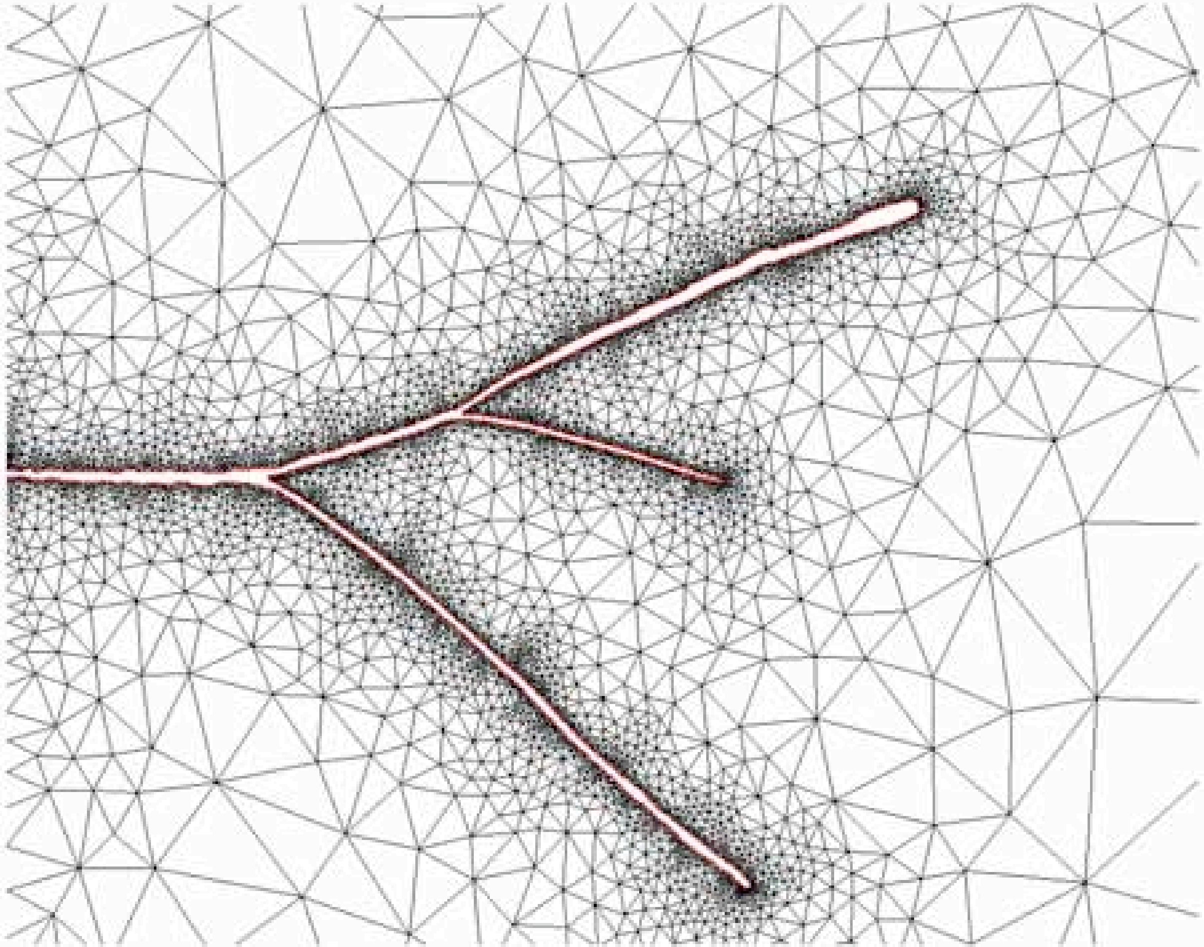

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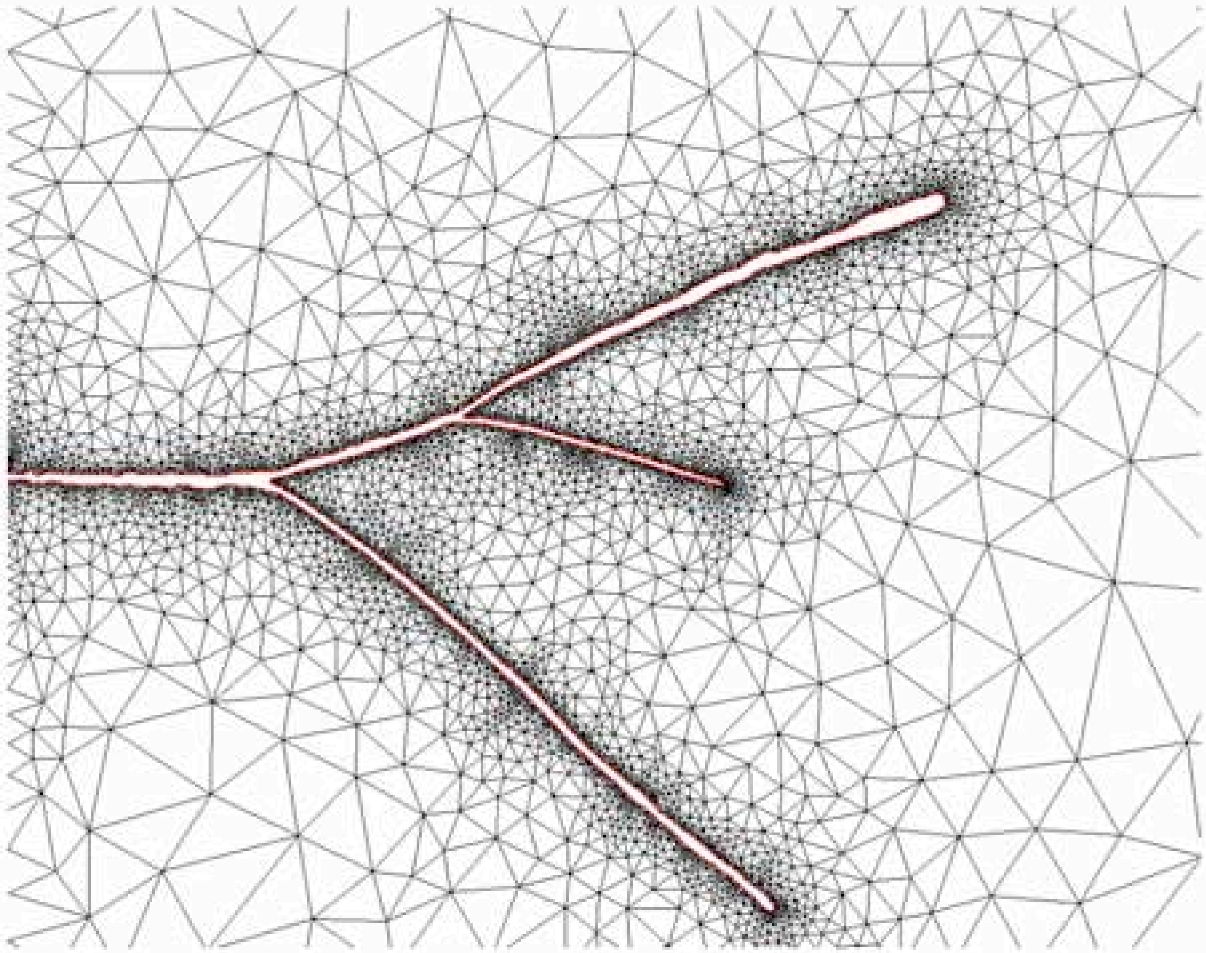

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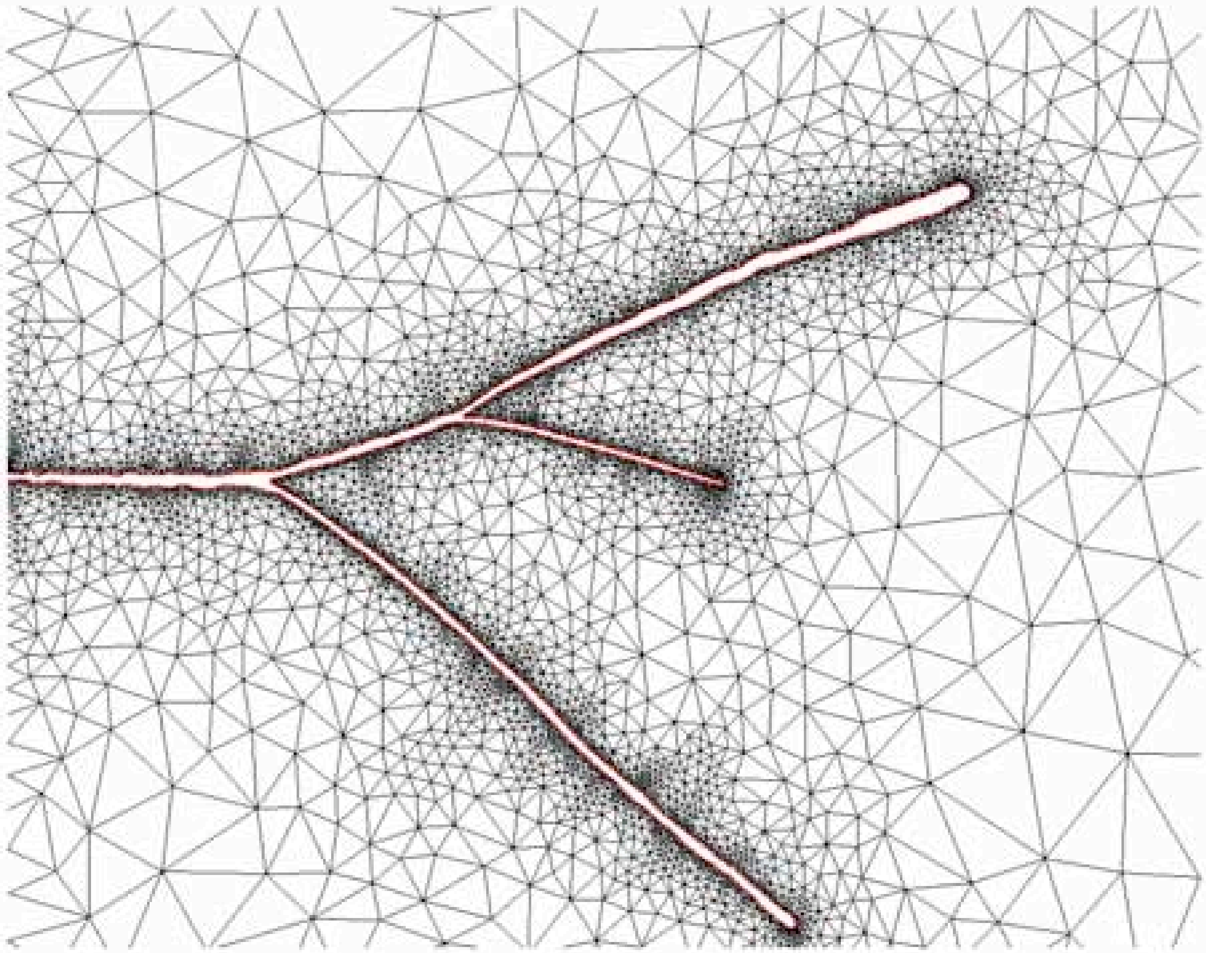

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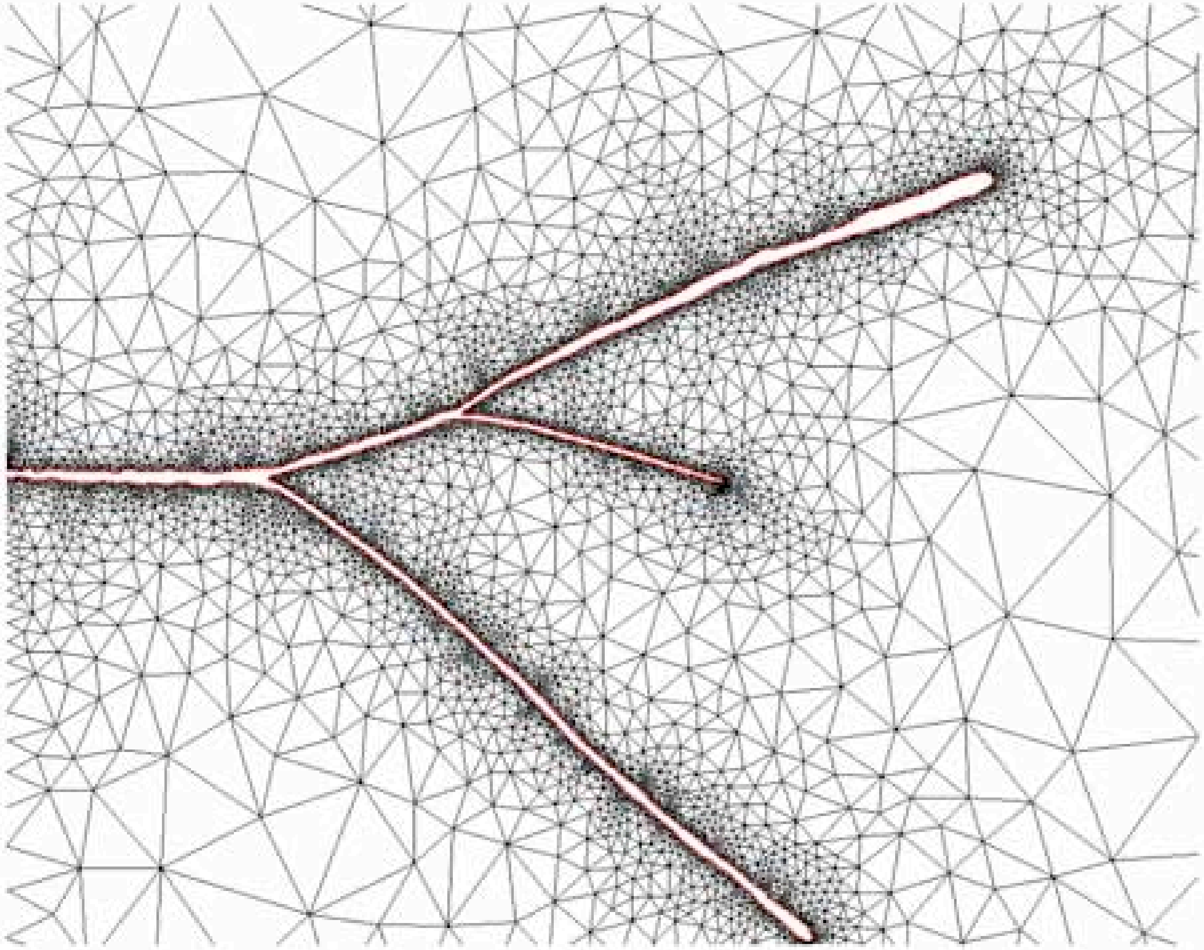

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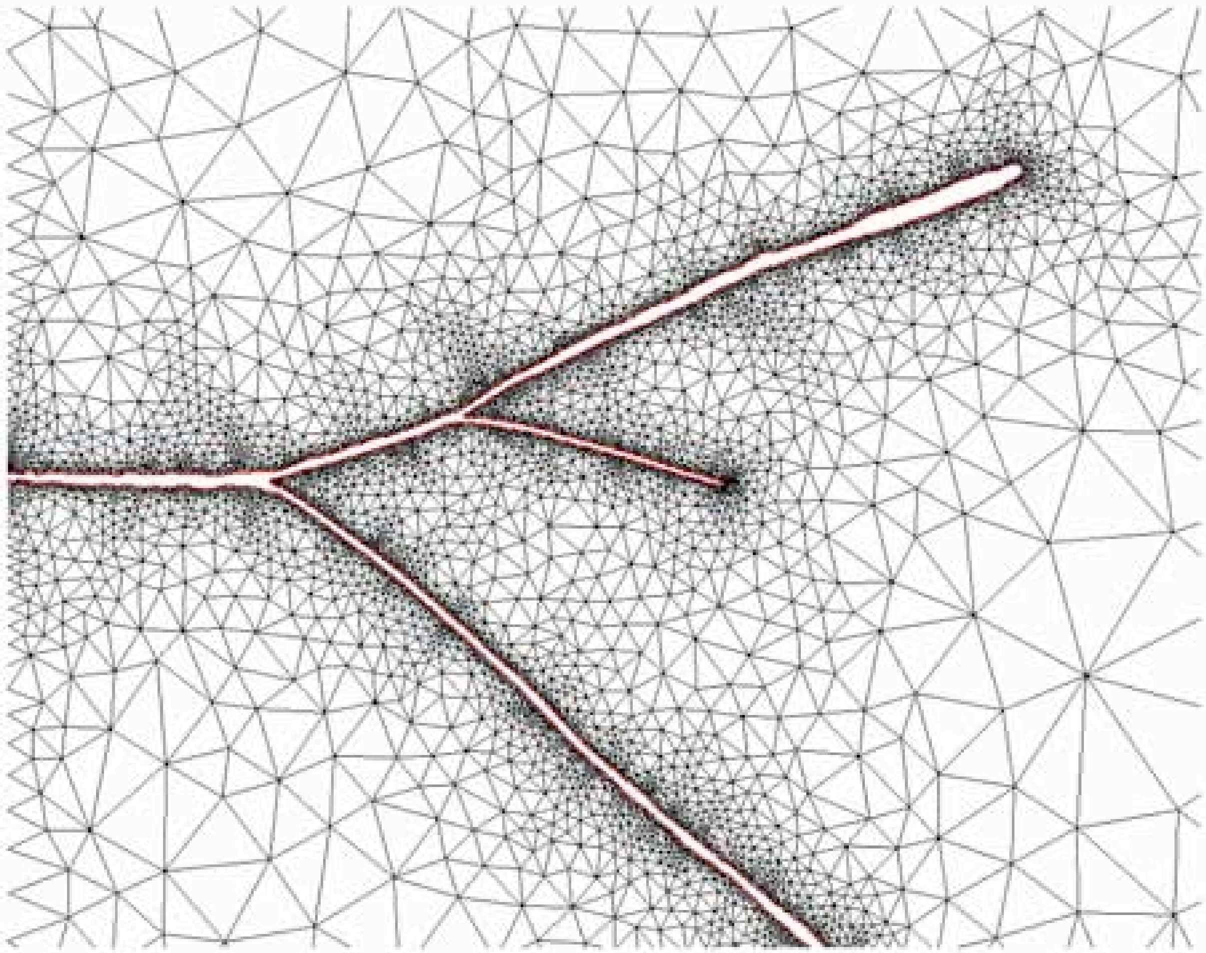

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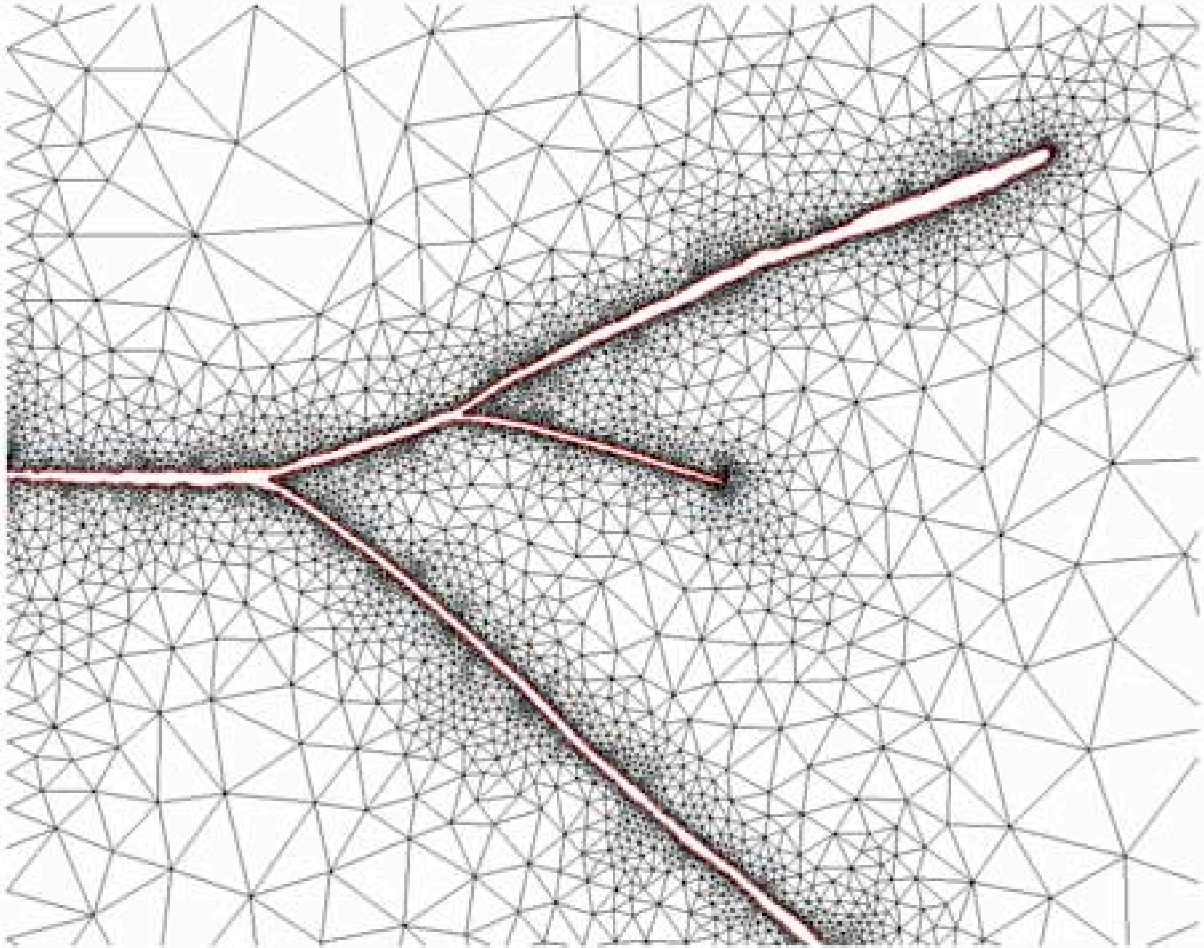

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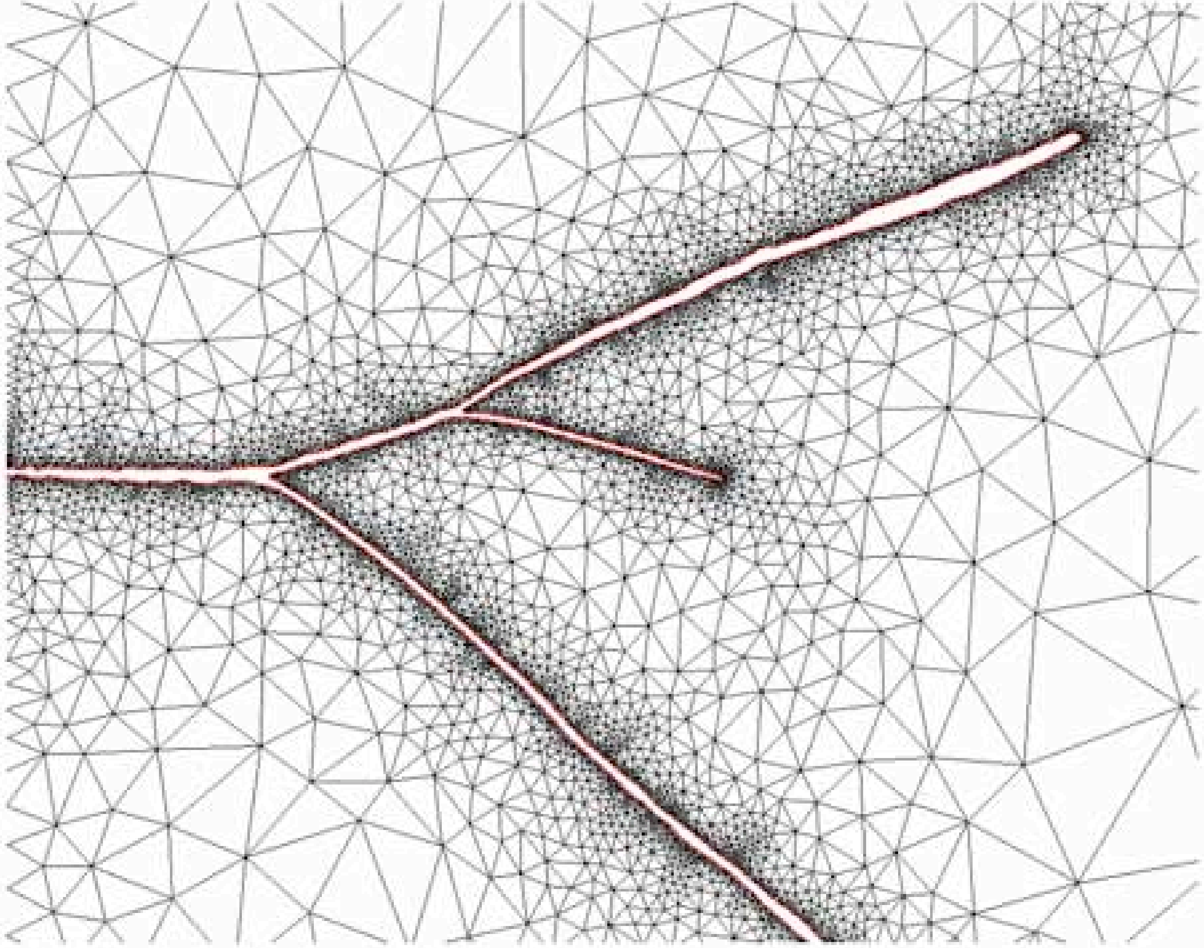

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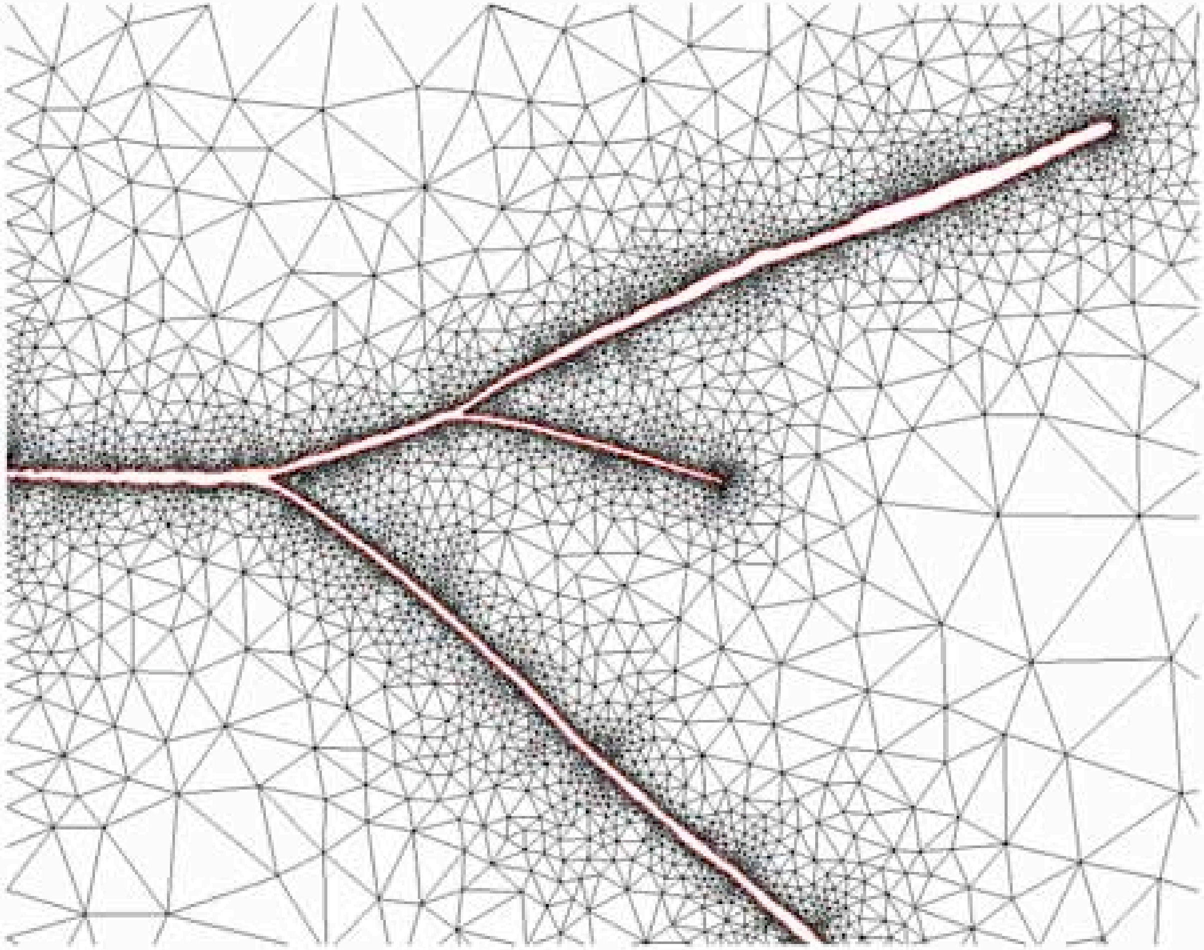

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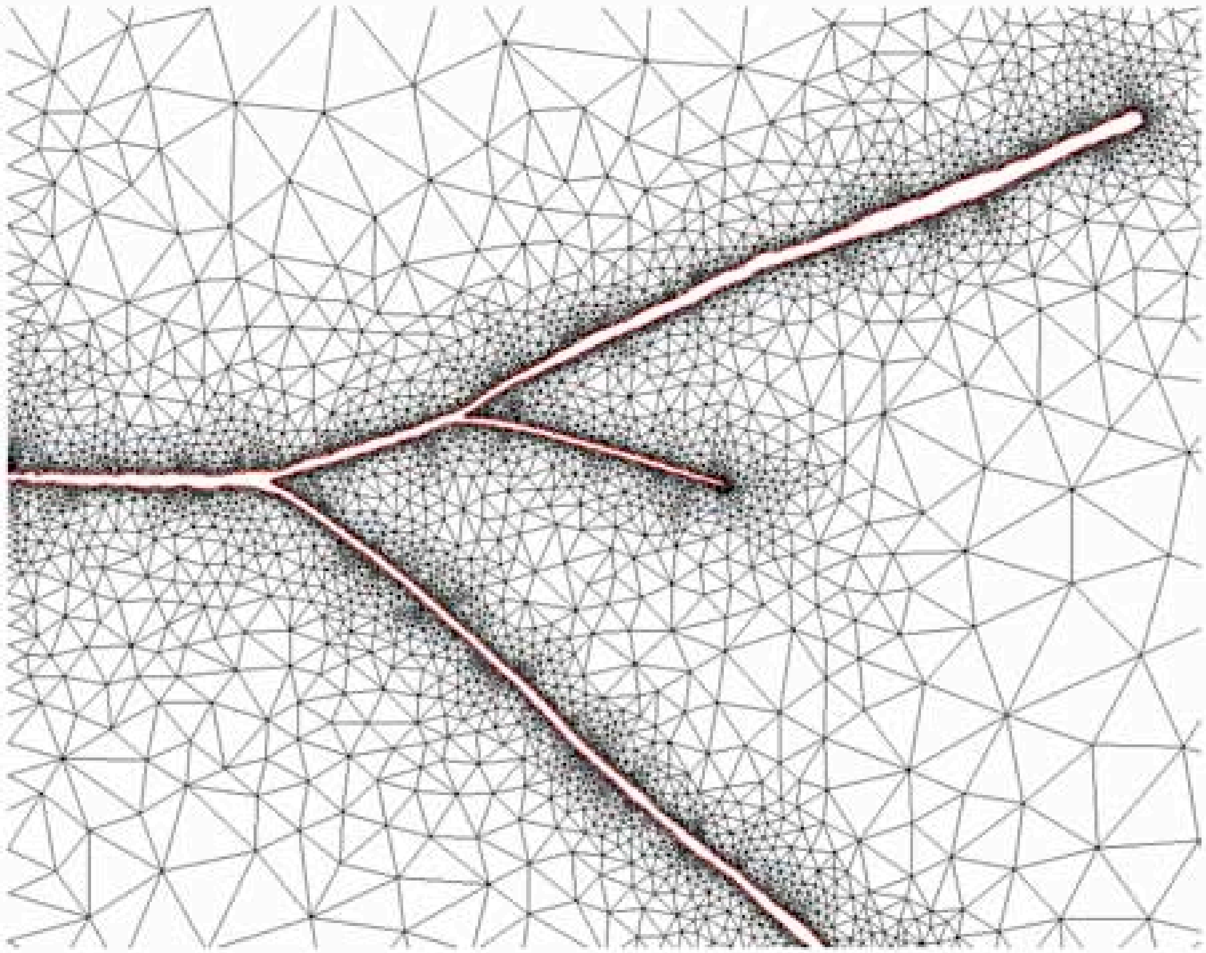

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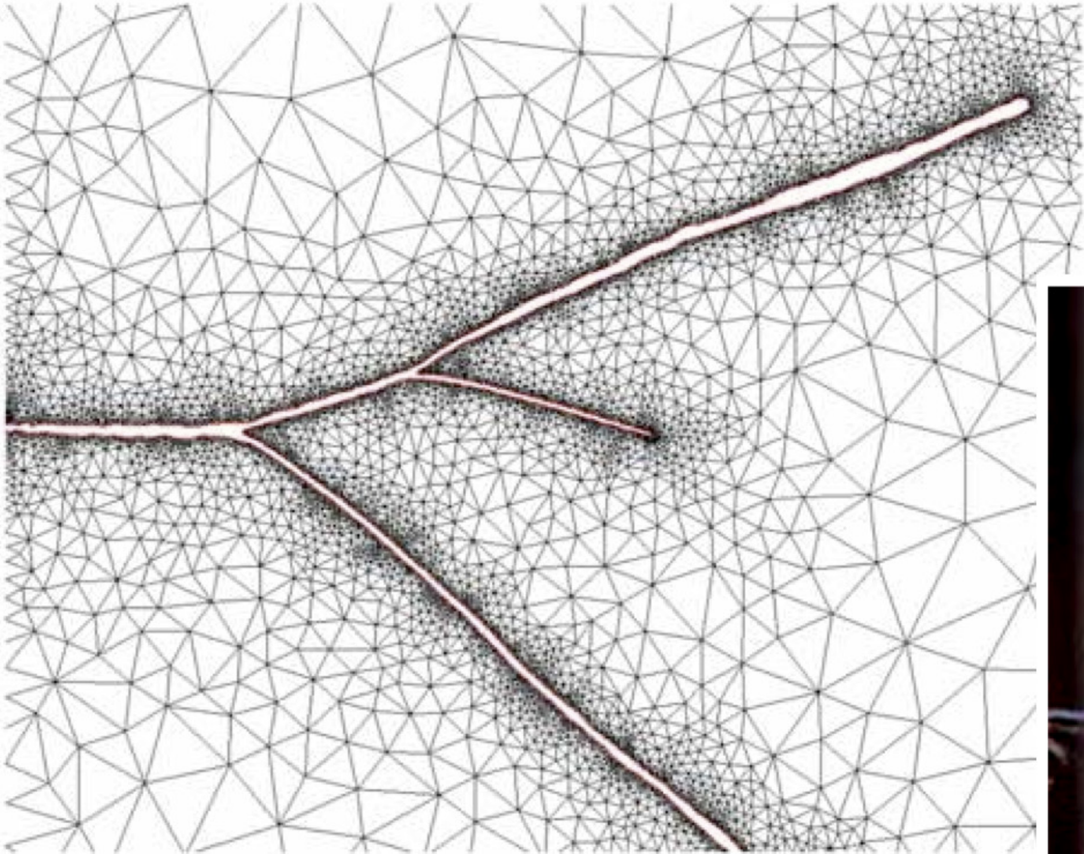
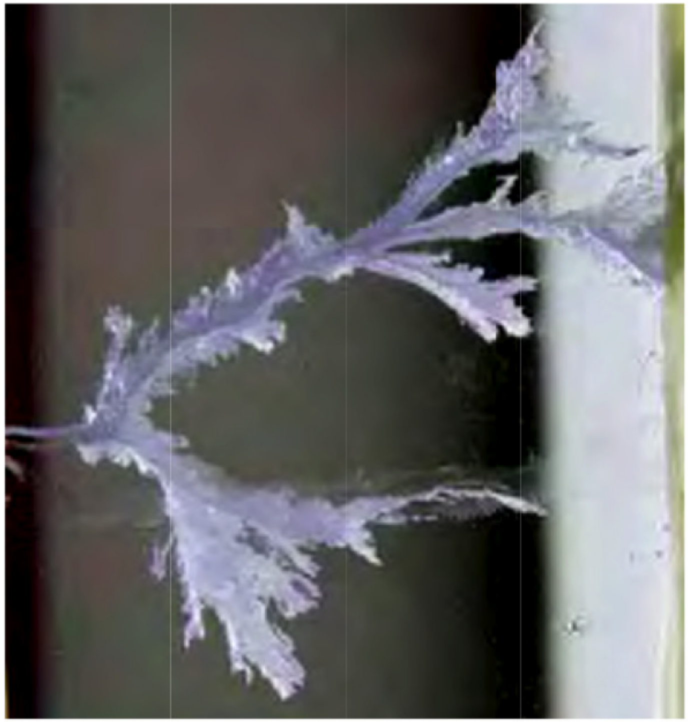
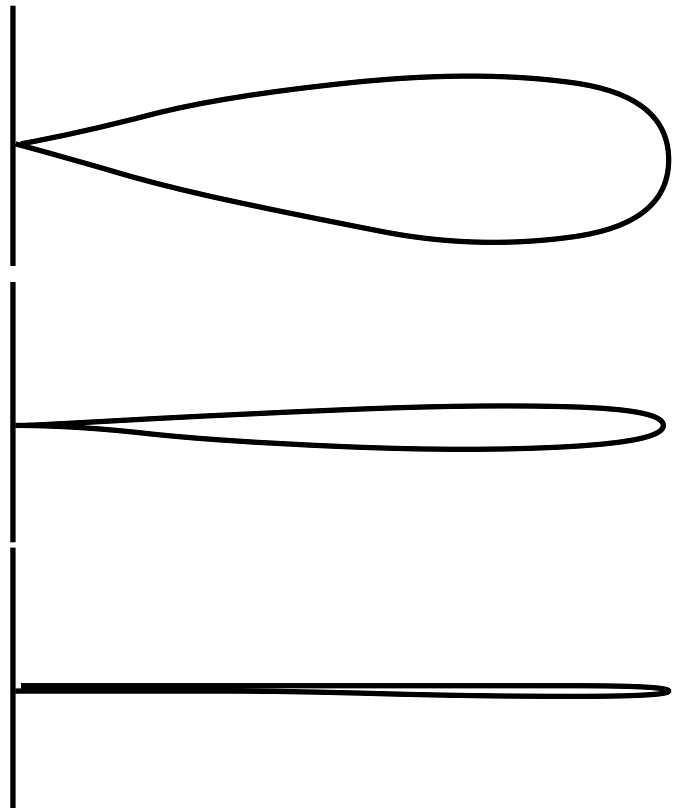
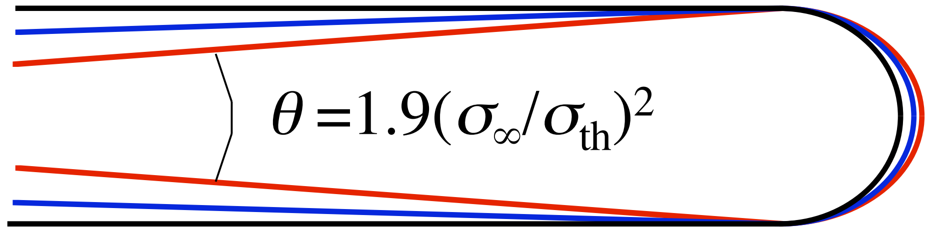
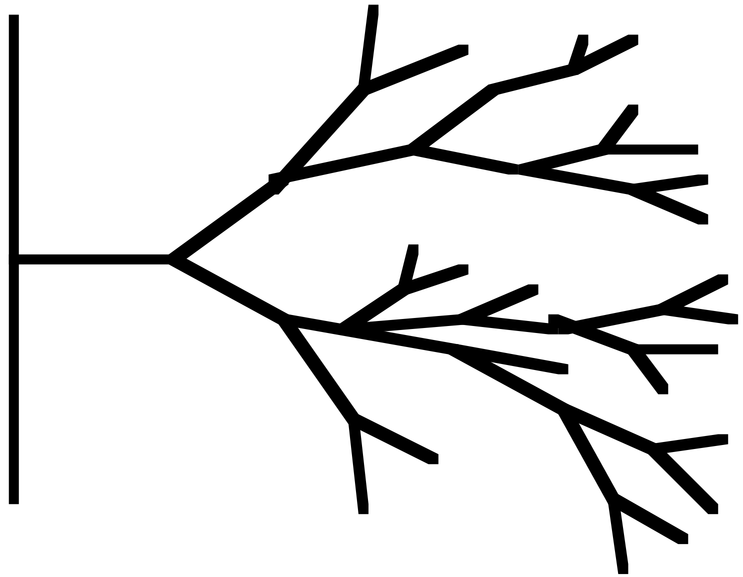




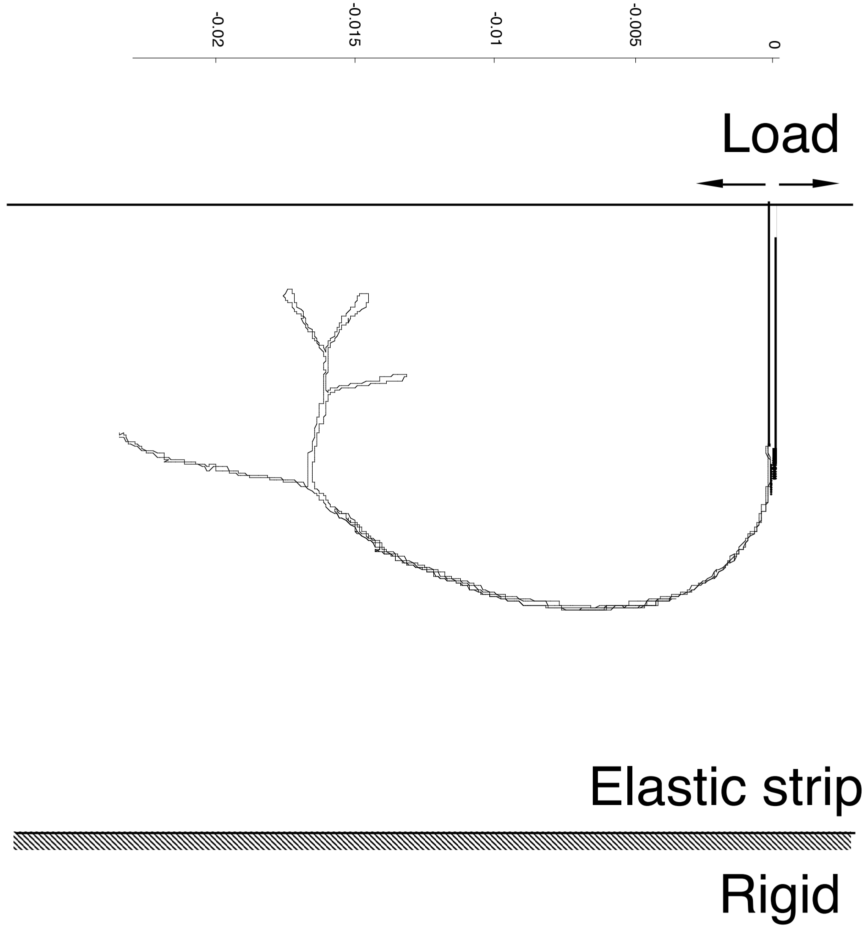
Missing lengthparameter => Selfsimilar growth

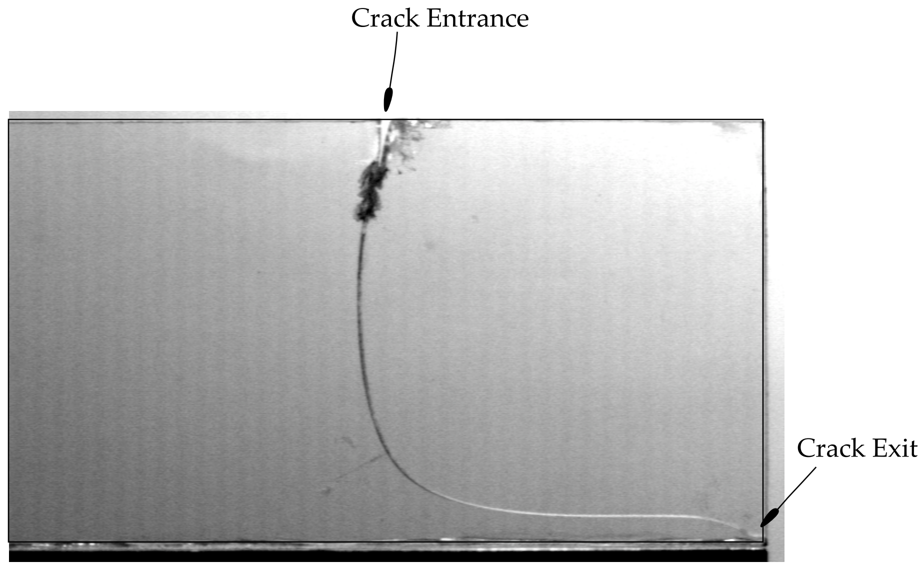




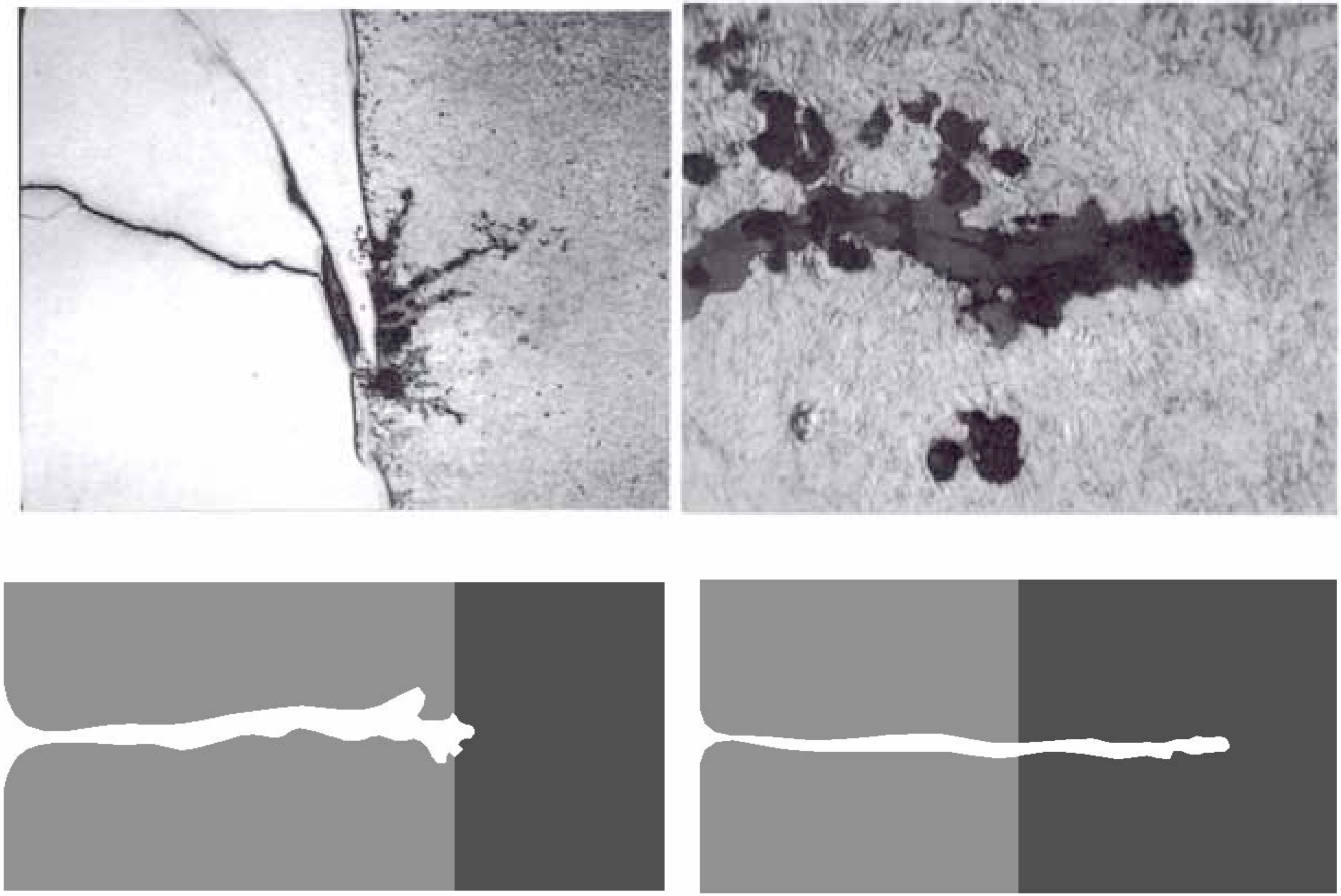


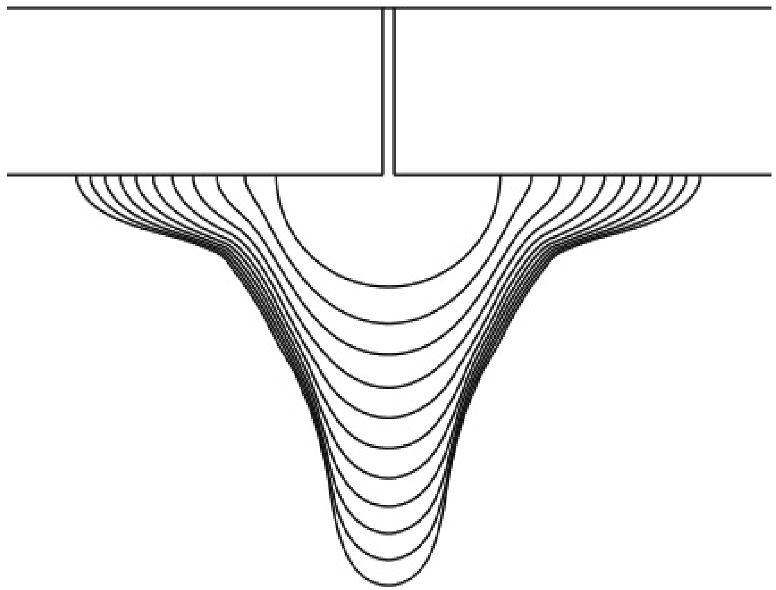
Crack seem to follow a mode I path

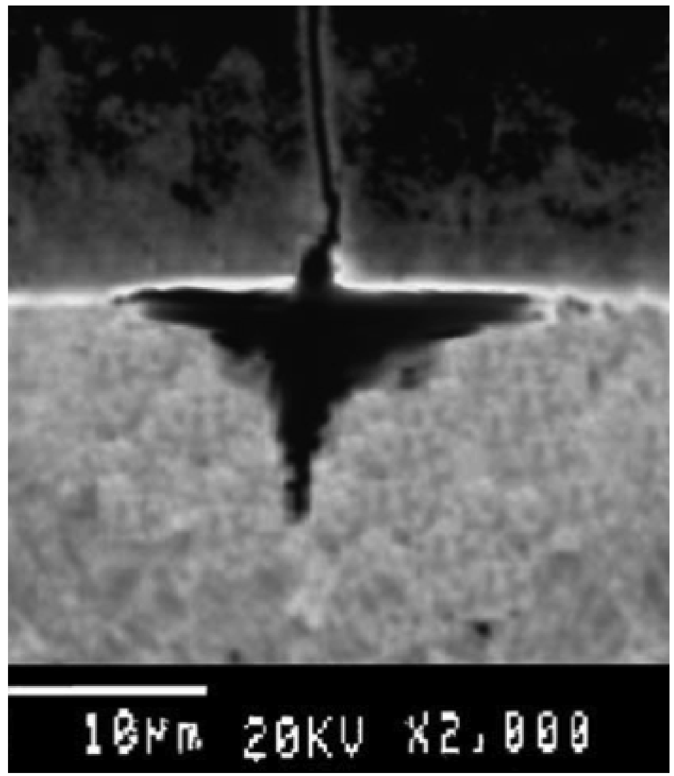




From Cladding to Grey Material



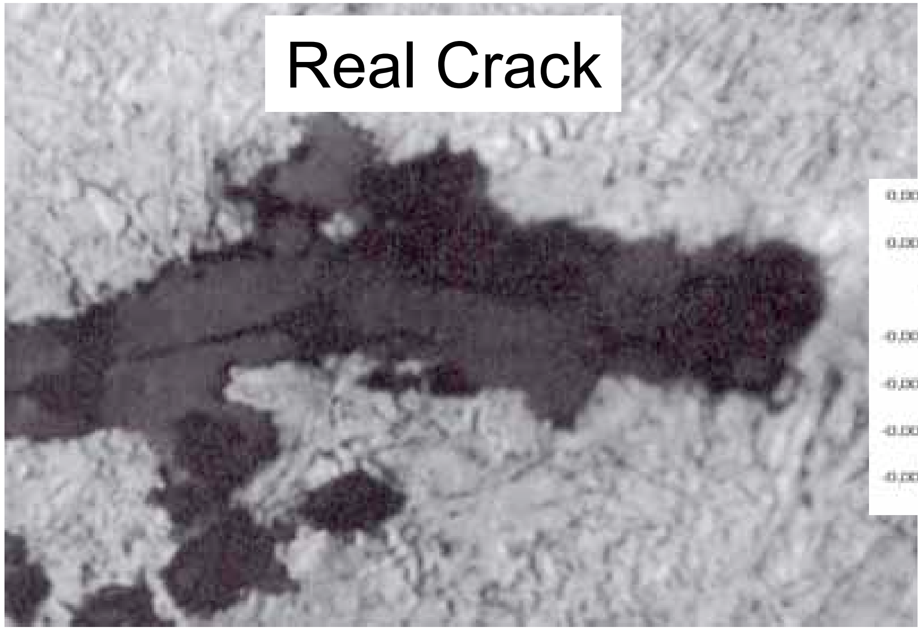




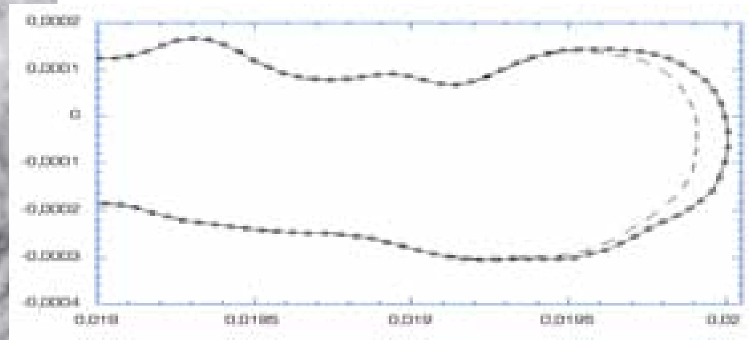
FEM simulation of material dissolution coating (Bjerkén and Ortiz, 2010)

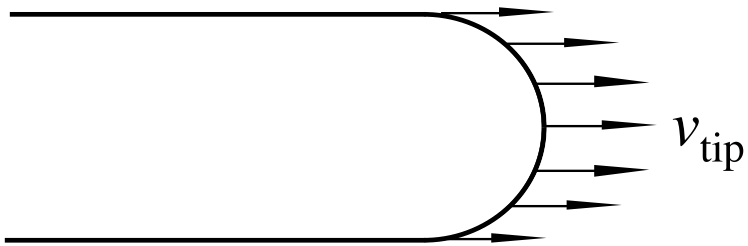
SEM observation of corrosion-erosion crack in a canon bore (Sopok et al. 2005)

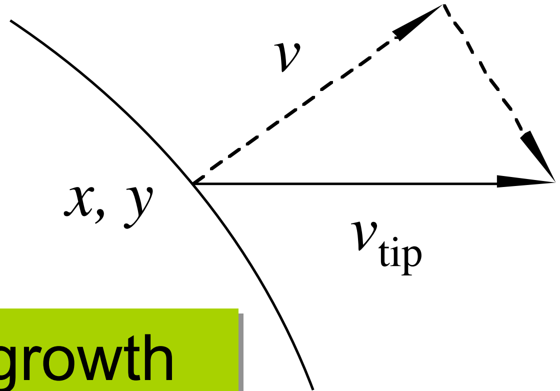
Steady State Crack-tip Shape



FEM result







Constant Component in the growth direction: $v = (x/\rho)\ v_{tip}$

Summary

Stress corrosion can be modelled as a moving bondary problem

Surface instability, formation cracks and crack growth are captured

Branching occurs as the blunted crack front become unstable

Phase field modelling simplifies the analysis

Time dependent solution to the Ginzburg-Landau equation found