Coupling of Water and Atmosphere Reactive Transport Simulations - the New 3D SMART Model

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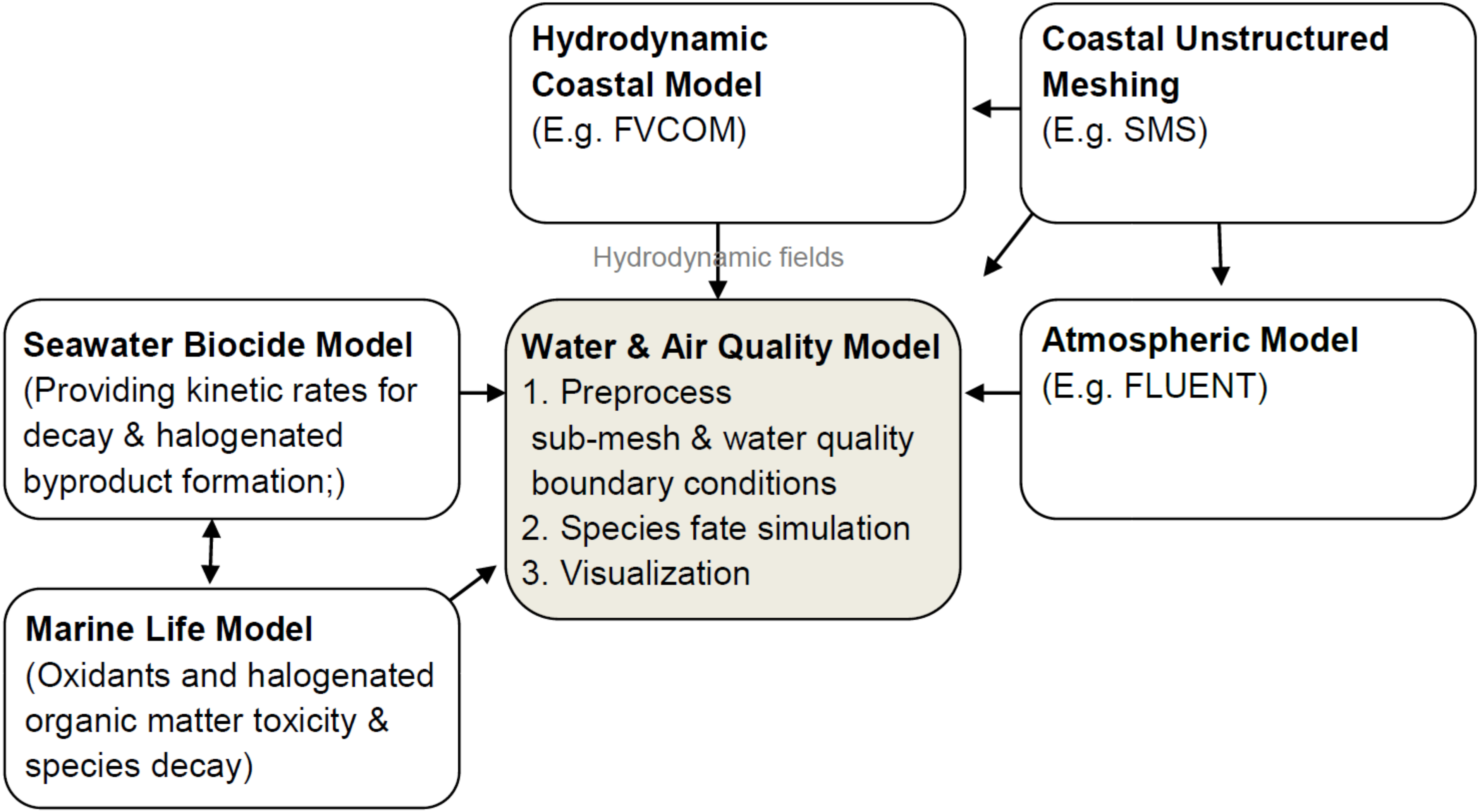
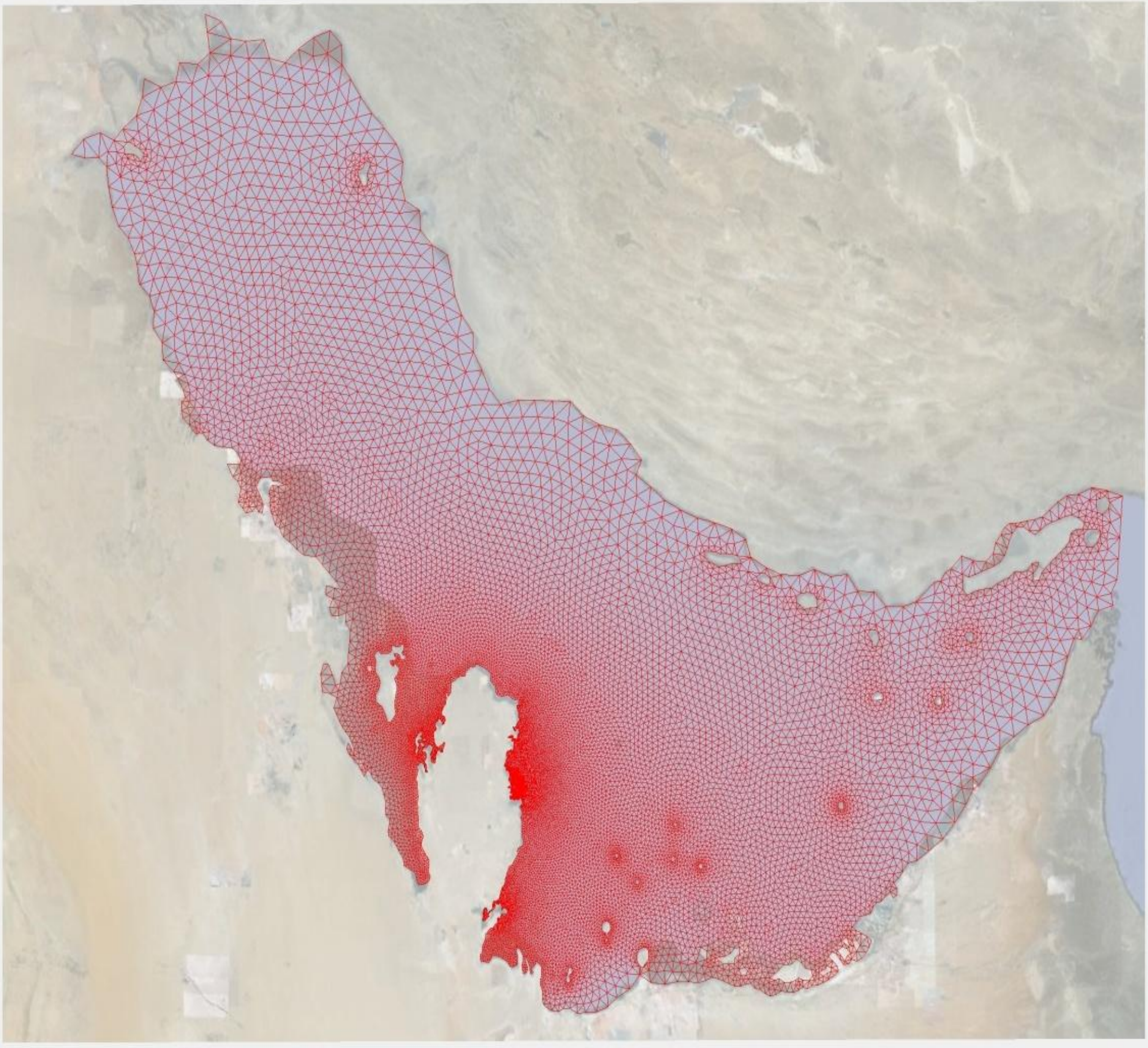

Hydrodynamic Coastal Model
(E.g. FVCOM)
Coastal Unstructured Meshing
(E.g. SMS)
Hydrodynamic fields
Seawater Biocide Model
(Providing kinetic rates for decay & halogenated byproduct formation;)
Water & Air Quality Model
1. Preprocess
sub-mesh & water quality boundary conditions
2. Species fate simulation
3. Visualization
Atmospheric Model
(E.g. FLUENT)
Marine Life Model
(Oxidants and halogenated organic matter toxicity & species decay)

Boundary Conditions

Boundary Condition with $\boldsymbol{n} \perp \partial\Omega$		FVE-approximation $\forall\, ihk$ corresponding to the BC
Horizontal Open	$0 = \left.\frac{\partial c}{\partial n}\right\vert_{n=0}$	$\pi_{ihs} = 0 \ \wedge \ g^t_{ihs} = 0$
No-flux	$0 = \boldsymbol{u}c - D\left.\frac{\partial c}{\partial n}\right\vert_{n=0}$	$\dot{v}^t_{ihs} = 0 \ \wedge \ g^t_{ihs} = 0$
Sea Boundary Layer	$c_w = \frac{c_{at}}{k_{eq}} \wedge \left.\frac{\partial c}{\partial z}\right\vert_{at\ intf} = 0$	$\boldsymbol{c}^{t+\Delta}_{h_{sea}} = \frac{\boldsymbol{c}^{t+\Delta}_{h_{air}}\boldsymbol{v}^t_{h_{air}} + \boldsymbol{c}^{t+\Delta}_{h_{sea}}\boldsymbol{v}^t_{h_{sea}}}{k_{eq}\boldsymbol{v}^t_{h_{air}} + \boldsymbol{v}^t_{h_{sea}}} \wedge \ \boldsymbol{g}^t_{h_{sea}s} = 0$
Air Boundary Layer	$c_w = \frac{c_{at}}{k_{eq}} \wedge \left.\frac{\partial c}{\partial z}\right\vert_{at\ intf} = 0$	$\boldsymbol{c}^{t+\Delta}_{h_{air}} = \frac{\boldsymbol{c}^{t+\Delta}_{h_{air}}\boldsymbol{v}^t_{h_{air}} + \boldsymbol{c}^{t+\Delta}_{h_{sea}}\boldsymbol{v}^t_{h_{sea}}}{\boldsymbol{v}^t_{h_{air}} + \frac{\boldsymbol{v}^t_{h_{sea}}}{k_{eq}}} \wedge \ \boldsymbol{g}^t_{h_{air}s} = 0$
Sea Boundary Layer with constituent in atmosphere	$c_w = \frac{c_{at}}{k_{eq}} \wedge \left.\frac{\partial c}{\partial z}\right\vert_{at\ intf} = 0$	$\boldsymbol{c}^{t+\Delta}_{h_{sea}} = \frac{c_{at}}{k_{eq}} \wedge \ \boldsymbol{g}^t_{h_{sea}s} = 0$
Vertical air BC at atmospheric top-layer	$D\left.\frac{\partial c}{\partial z}\right\vert_{z=0^-} = D\left.\frac{\partial c}{\partial z}\right\vert_{z=0}$	$\boldsymbol{c}^t_{q+1} = \boldsymbol{g}^t_{qs}\left(\boldsymbol{c}^t_q - \boldsymbol{c}^t_{q-1}\right) + \boldsymbol{c}^t_q$



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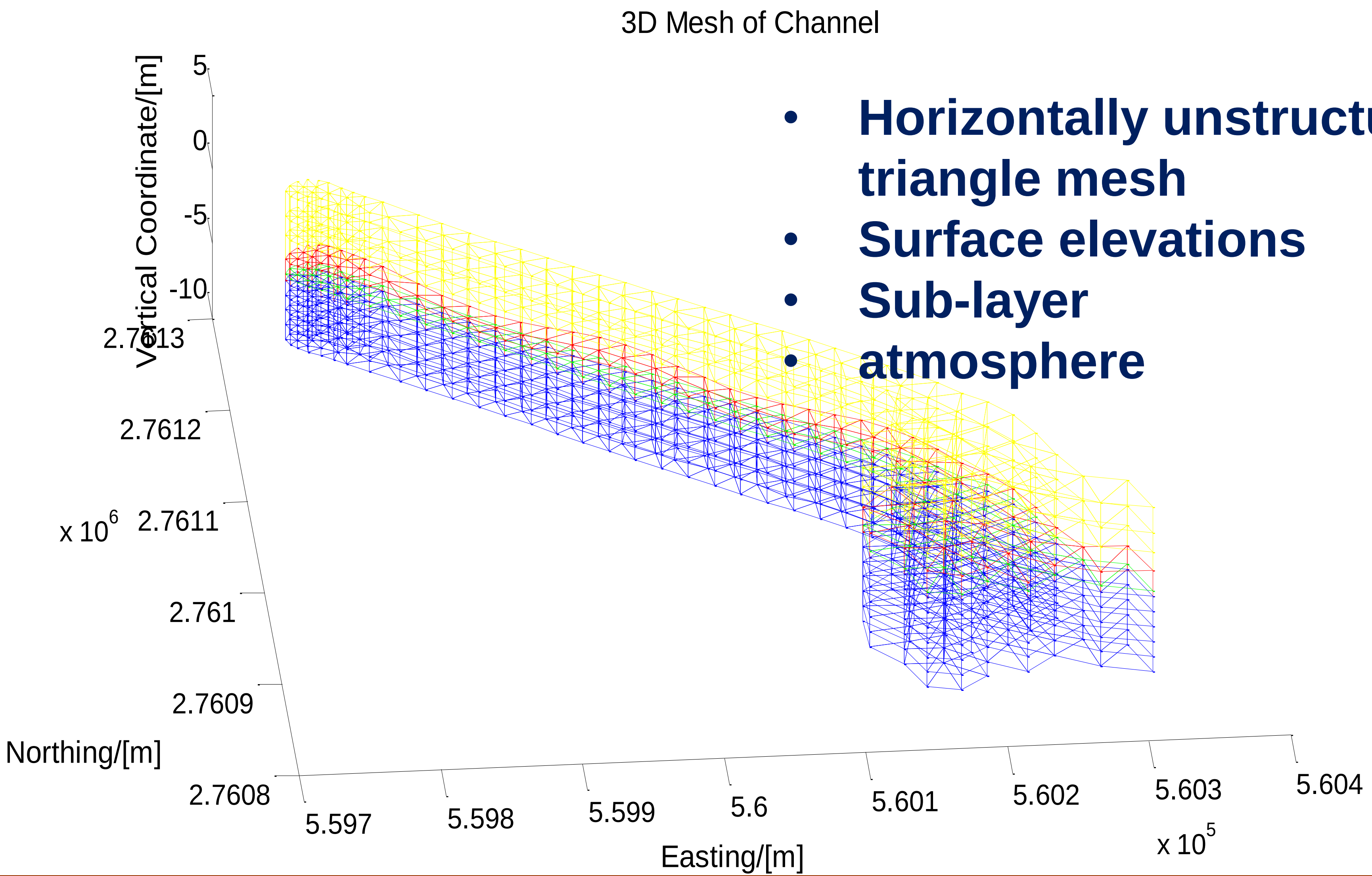
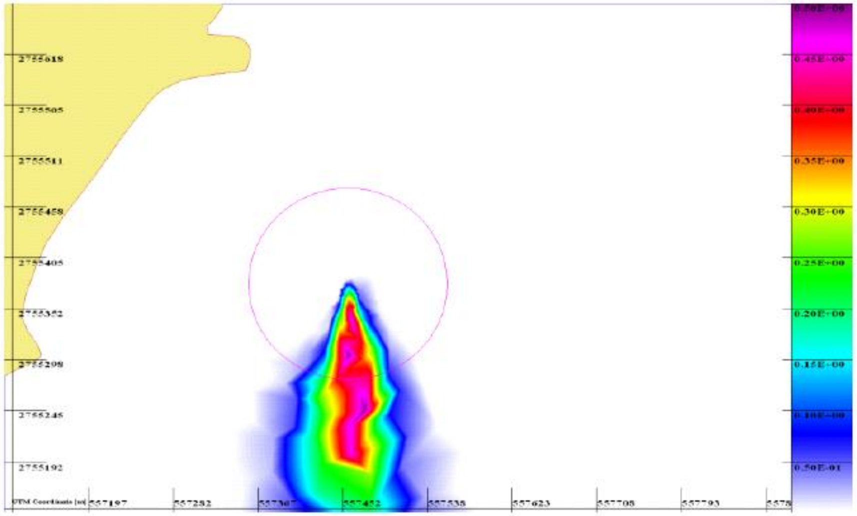
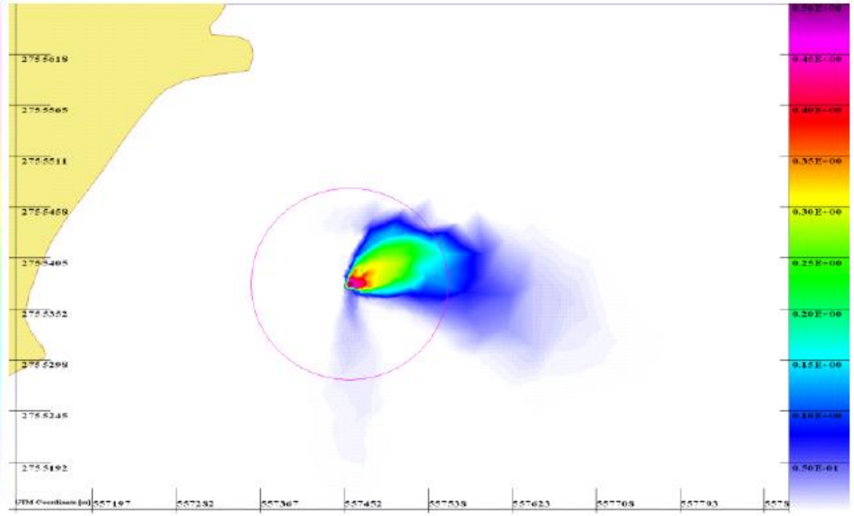


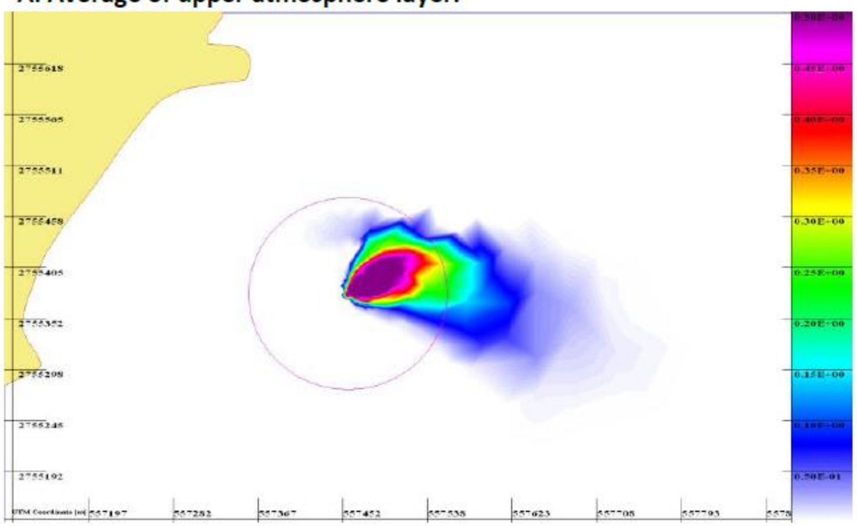
- **Horizontally unstructured triangle mesh**
- **Surface elevations**
- **Sub-layer**
- **atmosphere**



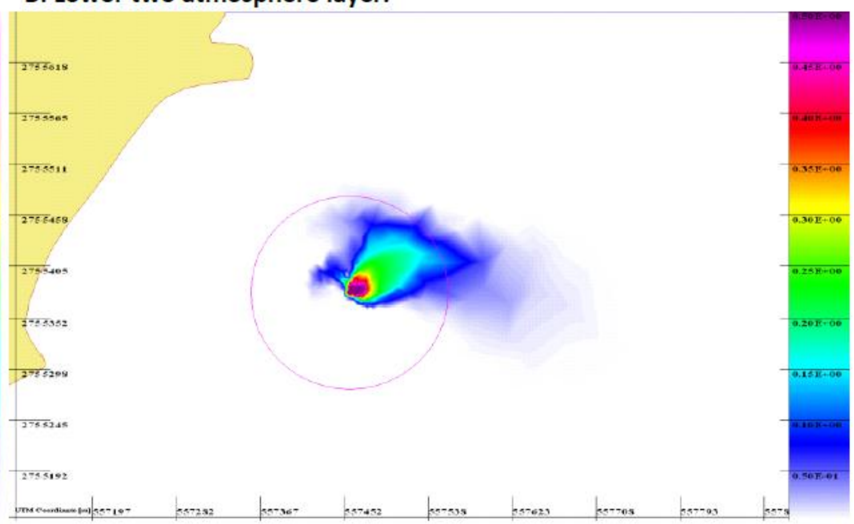
A: Average of upper atmosphere layer.



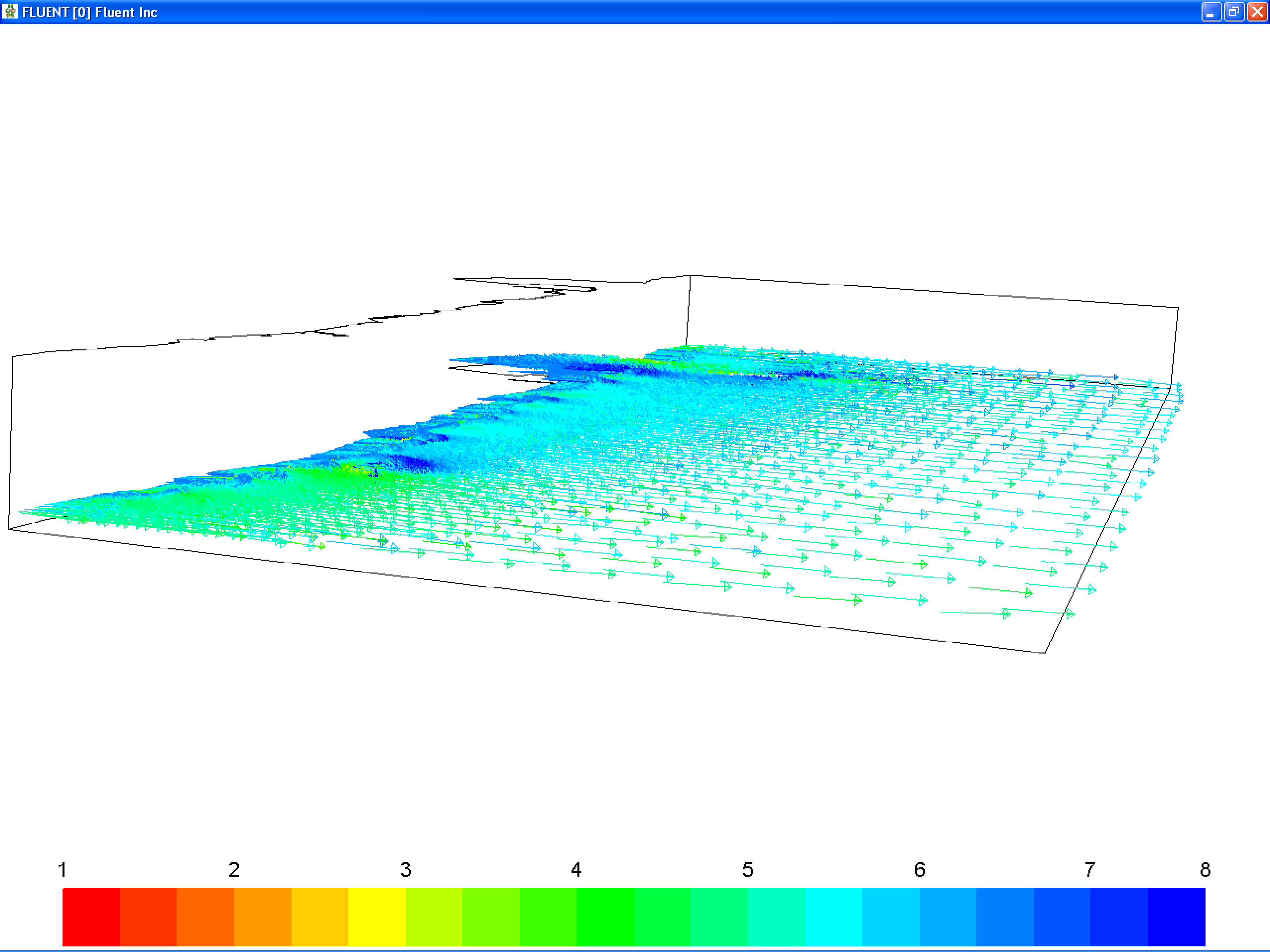
B: Lower two atmosphere layer.



C: Top-layer sea.



D: Average sea except top layer.


FLUENT [0] Fluent Inc
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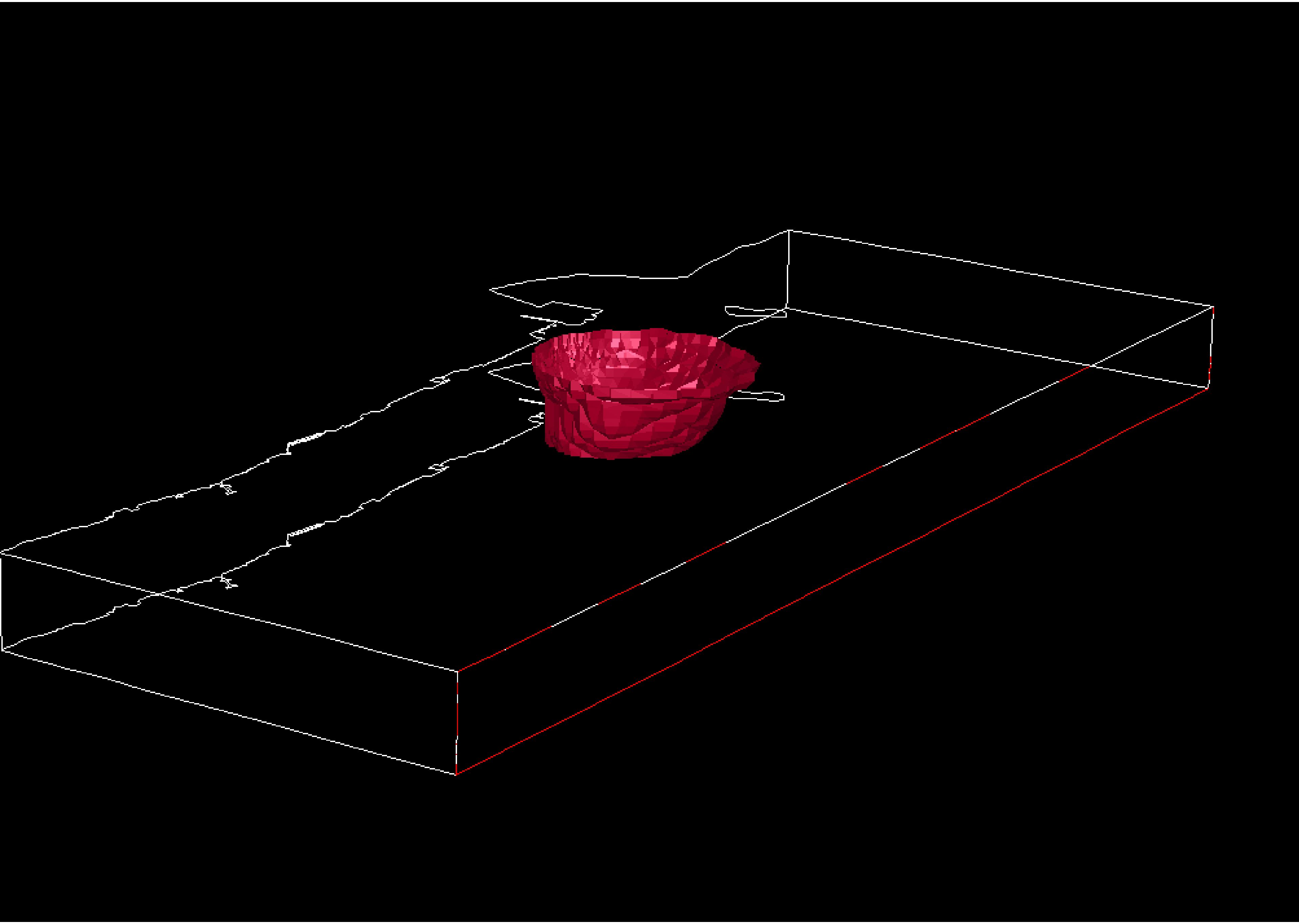

Precursor Simulations

Joint sea and atmosphere species transport precursor simulations are carried out as byproduct of existing projects:

- **Arabian Gulf model**

Conclusion

The 3D SMART is capable to simulate coupled sea-atmosphere natural gas plumes.

Identified Prerequisites

- **Calibrated Arabian Gulf model including all data (bathymetry, salinity fields, tidal data etc.)**
- **3 models coupled and ran on the same super computer**

This publication was made possible by NPRP grant # 29-6-7-39 from the Qatar National Research Fund (a member of Qatar Foundation). The statements made herein are solely the responsibility of the authors.