Fire Dynamics Simulator: Advances on simulation capability for complex geometry

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- Defining cut-cells: Computational geometry.
- Scalar transport near internal boundaries.
- The energy equation, thermodynamic divergence constraint.
- Reconstruction for momentum equations. Divergence equivalence.
- Poisson equation.
- Examples.
- Future work.

Motivation, Objective

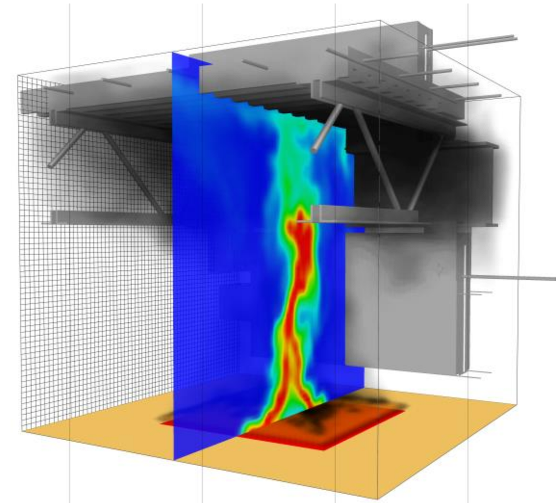
The Fire Dynamics Simulator* (FDS) is used in:

- performance-based design of fire protection systems,
- forensic work,
- Simulation of wild land fire scenarios.

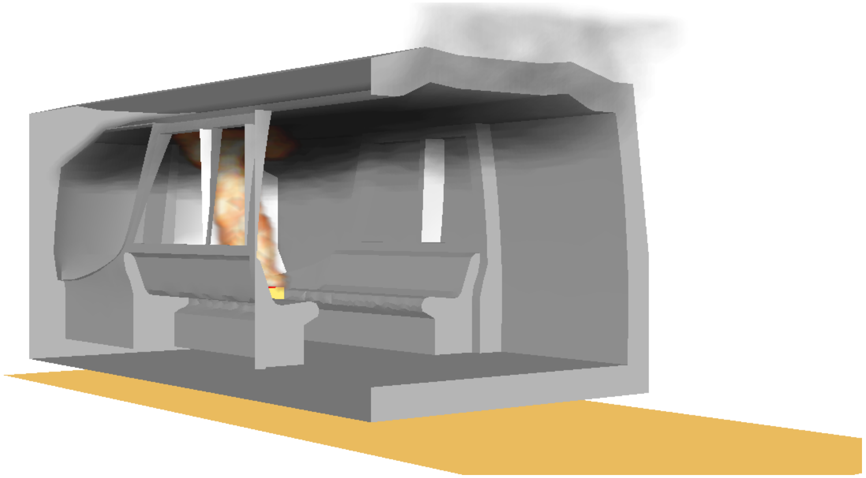
Uses block-wise structured, rectilinear grids for gas phase, and “lego-block” geometries to represent internal boundaries.

Objective:

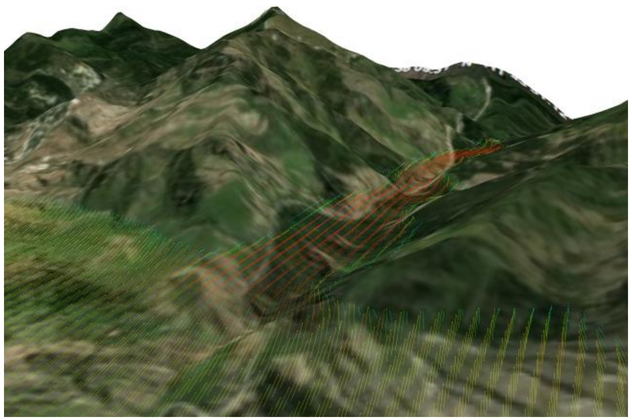
- Develop an efficient, conservative numerical scheme for treatment of complex geometry within FDS.



Fire-Structure Interaction: 12 MW fire load on a steel/concrete floor connection assembly.



LES of 800 KW propane fire in open train cart. Geometry courtesy of Fabian Braennstroem (Bombardier).



Velocity vectors (35 m/s [78 mph] max [red]) for a wind field in Mill Creek Canyon, Utah.
4 km x 4 km horizontal domain, 1 km vertical.
40 m grid resolution on a single mesh.

* K. McGrattan et al. Fire Dynamics Simulator, Tech. Ref. Guide, NIST. Sixth Ed., Sept. (2013).

Motivation, Objective

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Spatial discretization and time marching in FDS, work areas:

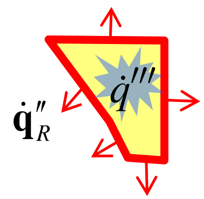
Scalar transport

$$\frac{\partial \rho Y_\alpha}{\partial t} + \nabla\cdot\left(\rho Y_\alpha \mathbf{u}\right) = -\nabla\cdot\left(-\rho D_\alpha \nabla Y_\alpha\right) + \dot{m}_\alpha''' \longrightarrow \rho^{n+1}, Y_\alpha^{n+1}$$

EOS

$$\bar{W}^{n+1} = \left[\sum_{\alpha=1}^{n_\alpha} Y_\alpha^{n+1} / W_\alpha\right]^{-1}, \quad T^{n+1} = \frac{\bar{p}\bar{W}^{n+1}}{\rho^{n+1}R} \longrightarrow T^{n+1}$$

Combustion, Radiation



Divergence Constraint*

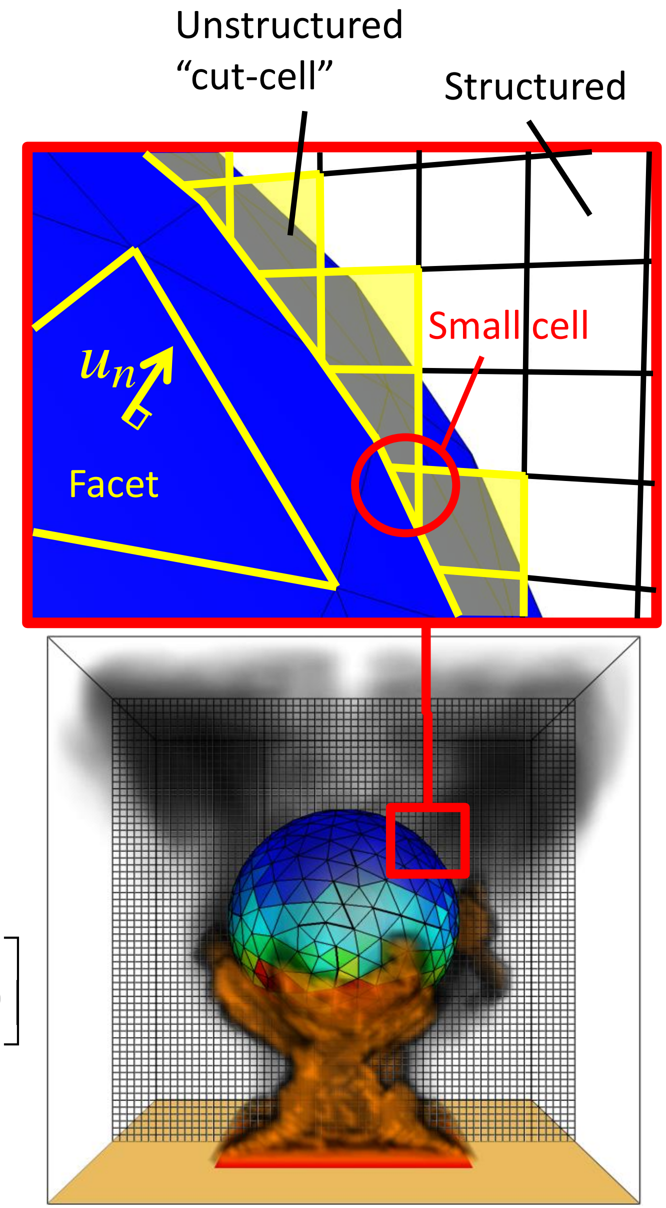
$$\nabla\cdot\mathbf{u} = \frac{1}{\rho h_s}\left[\frac{D}{Dt}\left(\bar{p} - \rho h_s\right) + \dot{q}''' - \nabla\cdot\dot{\mathbf{q}}''\right] \longrightarrow \left(\nabla\cdot\mathbf{u}\right)^{n+1}$$

Momentum + IBM⁺

$$\frac{\partial \mathbf{u}}{\partial t} = -\left(\mathbf{F} + \nabla H^{n-1}\right) \longrightarrow \mathbf{F}_{IB} = -\left(\frac{\partial \mathbf{u}}{\partial t}\right)_D - \nabla H^{n-1}$$

$$\frac{\partial}{\partial t}\left(\nabla\cdot\mathbf{u}\right) \approx \frac{\left(\nabla\cdot\mathbf{u}\right)^{n+1} - \nabla\cdot\mathbf{u}^n}{\Delta t}, \quad \Delta H = -\left[\nabla\cdot\mathbf{F} + \frac{\partial}{\partial t}\left(\nabla\cdot\mathbf{u}\right)\right]$$

$$\frac{\partial \mathbf{u}}{\partial t} = -\left(\mathbf{F} + \nabla H\right) \longrightarrow \mathbf{u}^{n+1} \quad \Delta H^n$$

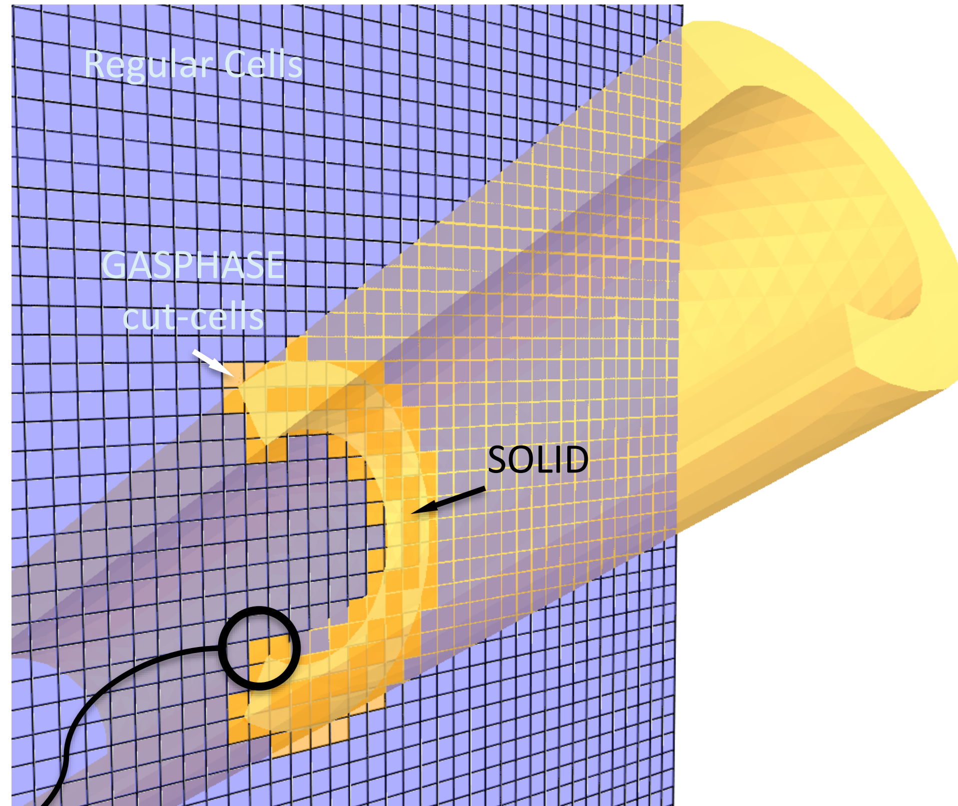


* R. J. McDermott. J. Comput. Phys. 274, pp. 413-431 (2014); + E. A. Fadlun et al. J. Comput. Phys. 161, pp. 35-60 (2000).

Computational Geometry

Objective:

- Define cut-cell volumes of Cartesian cells intersected by body.
- Robust, general, parallelizable.
- Ideally efficient for moving object problem.



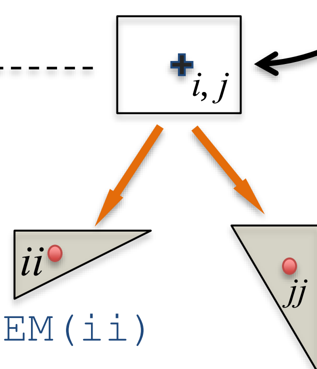
Smokeview Visualization inclined C-beam mid-plane. Obtained with computational geometry engine in FDS.

Data Management:

- Work by Eulerian mesh block. Body surfaces defined by triangulations.
- Hierarchical data structures are defined, capable of arbitrary number of cut-faces and cut-cells per Cartesian counterparts.

- Cartesian Level -----------------
`IBM_CUTCELL(m)`

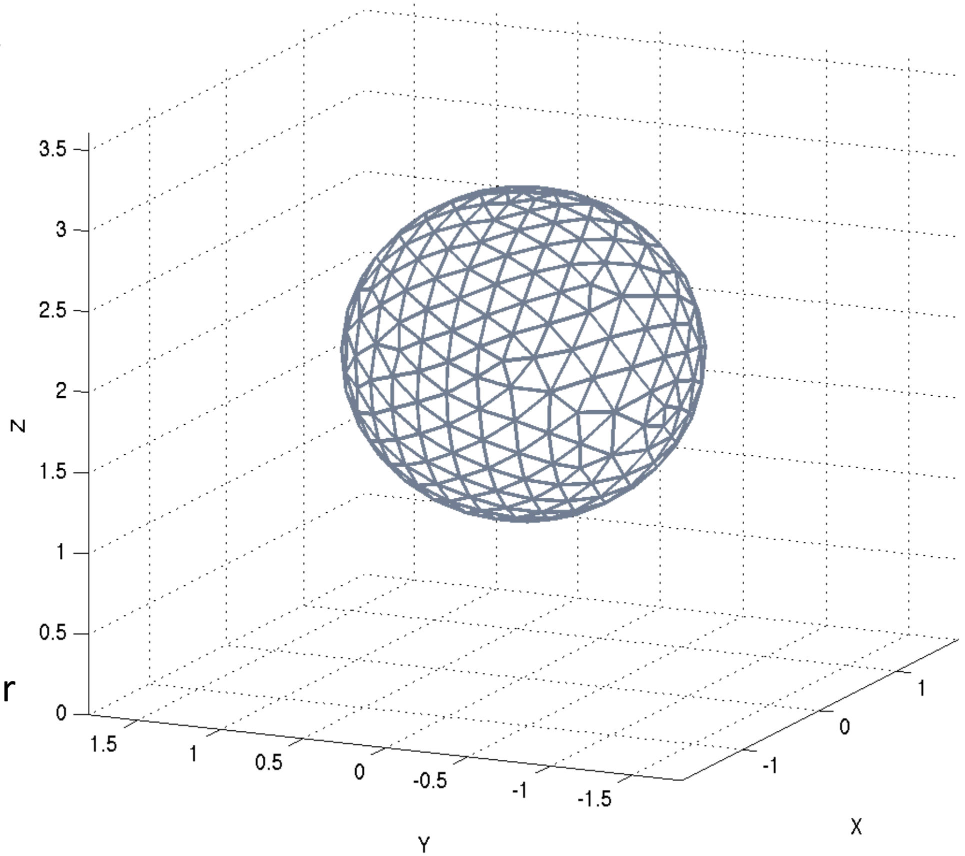
- Cut-cell Level ----------
`IBM_CUTCELL(m)%CCELEM(ii)`



Computational Geometry

Scheme:

- Body-plane intersection elements (segments, triangles) are defined for all Cartesian grid planes. Intersections along surface triangles also defined.
- Cut-faces on Cartesian planes are defined by joining segments. Same for cut-faces along triangles.
- Working by Cartesian cell, cut face sets are found for each **cut-cell** volume.
- Area and volume properties are computed for each cut-face and cell.
- Interpolation stencils are found for centroids (IBM).



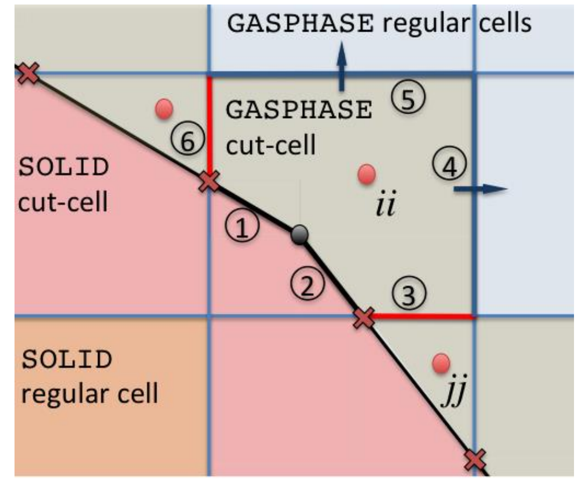
Cut-cell definition on original Matlab implementation.

Scalar Transport

Based on mass fractions: $\dfrac{\partial \rho Y_\alpha}{\partial t} + \nabla \cdot \left(\rho Y_\alpha \mathbf{u} \right) = -\nabla \cdot \mathbf{J}_\alpha + \dot{m}_\alpha''' \;\; ; \;\; \alpha = 1, \ldots, N$ on domain + Ics, Bcs

Take: $$\mathbf{J}_a = - r D_a \nabla Y_a = - \left(D_a \nabla (r Y_a) - \frac{D_a}{r} \nabla r \;\; (r Y_a) \right)$$

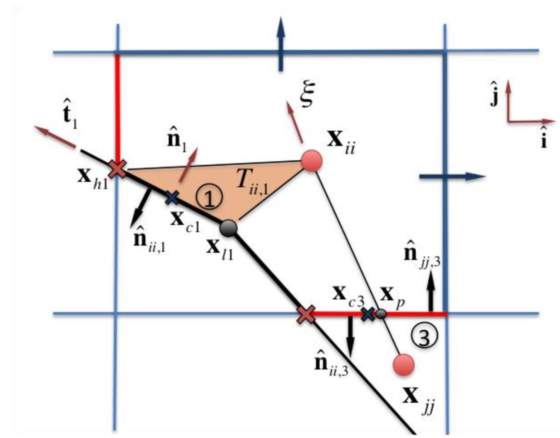
Then:
$$\frac{\partial \rho Y_\alpha}{\partial t} + \nabla \cdot \left(\mathbf{u}' \rho Y_\alpha \right) = \nabla \cdot \left(D_\alpha \nabla (\rho Y_\alpha) \right) + \dot{m}_\alpha''' \;\; ; \;\; \mathbf{u}' = \mathbf{u} + \frac{D_\alpha}{\rho} \nabla \rho$$



Finite Volume method: Divide the domain on $ii \rightarrow (i,j) \in \Im$ cells.

- **Advection:**

$$\int_{W_{ii}} \nabla \cdot \left(\mathbf{u}' r Y_a \right) dW = \int_{\partial W_{ii}} \left(\mathbf{u}' r Y_a \right) \cdot \hat{\mathbf{n}}_{ii} d\partial W = \sum_{k=1}^{nfc} \left(\mathbf{u}' r Y_a \right)_k \cdot \hat{\mathbf{n}}_{ii,k} A_k$$



For a given face (k=4, cut-cell *ii*):

$$\left(\mathbf{u}' r Y_a \right)_k \times \hat{\mathbf{n}}_{ii,k} A_k = \left[\overline{\left(r Y_a \right)}_k^{fl} \mathbf{u}_k + \overline{\left(r Y_a \right)}_k^{lin} \left(\frac{D_a}{r} \nabla r \right)_k \right] \cdot \hat{\mathbf{n}}_{ii,k} A_k$$

- **Diffusion:** $$\int_{W_{ii}} \nabla \cdot \left(D_a \nabla (r Y_a) \right) dW = \int_{\partial W_{ii}} \left(D_a \nabla (r Y_a) \right) \cdot \hat{\mathbf{n}}_{ii} d\partial W = \sum_{k=1}^{nfc} \left(D_a \nabla (r Y_a) \right)_k \cdot \hat{\mathbf{n}}_{ii,k} A_k$$

Scalar Transport

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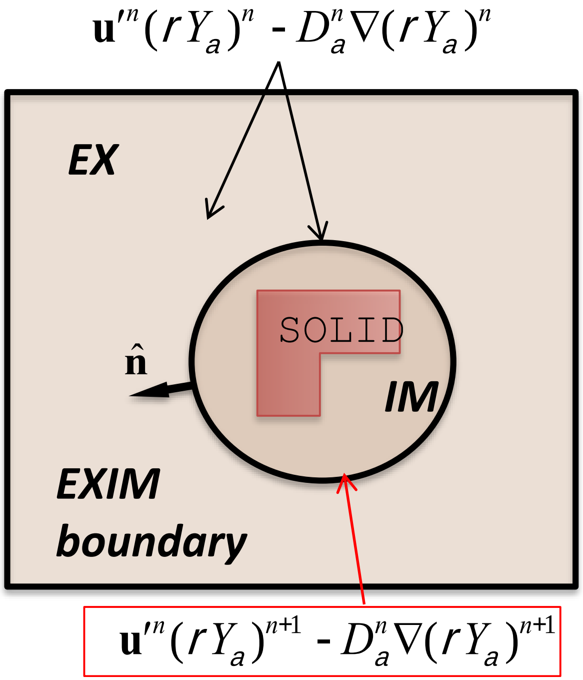
- Small cut-cells are problematic for explicit time integration.
- Alleviation methods tend to be arbitrary, deteriorating the solution quality.



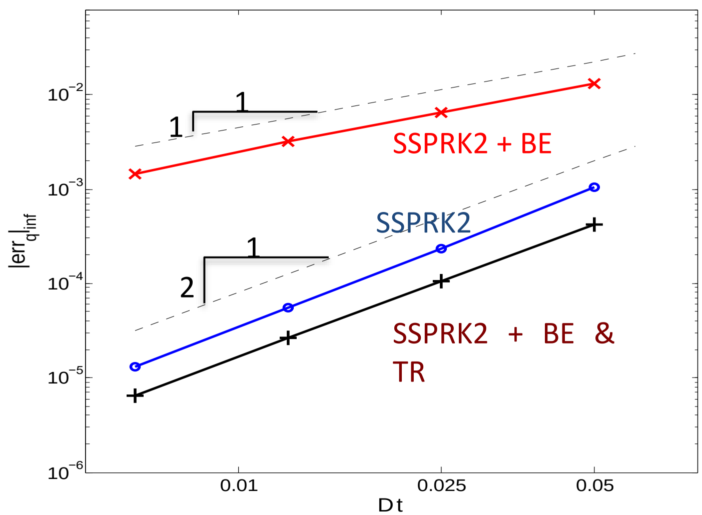
Explicit - Implicit time integration*:

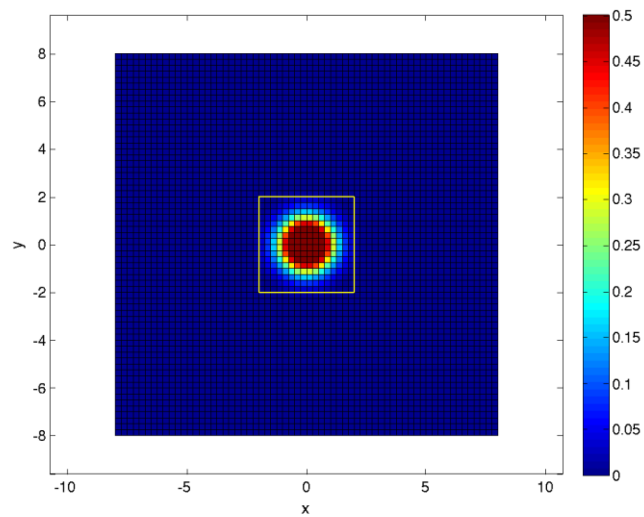
- **Explicit region**: Advance first.
- **Implicit region**: linearizing transport, i.e. implicit BE:

$$\frac{(\rho Y_a)^{n+1} - (\rho Y_a)^n}{\Delta t} = -\nabla\cdot\left(\boxed{\mathbf{u}'^n(\rho Y_a)^{n+1} - D_a^n\nabla(\rho Y_a)^{n+1}}\right)$$

*- C.N. Dawson, T.F. Dupont. SIAM J. Numer. Analysis 31:4, pp. 1045-1061 (1994).

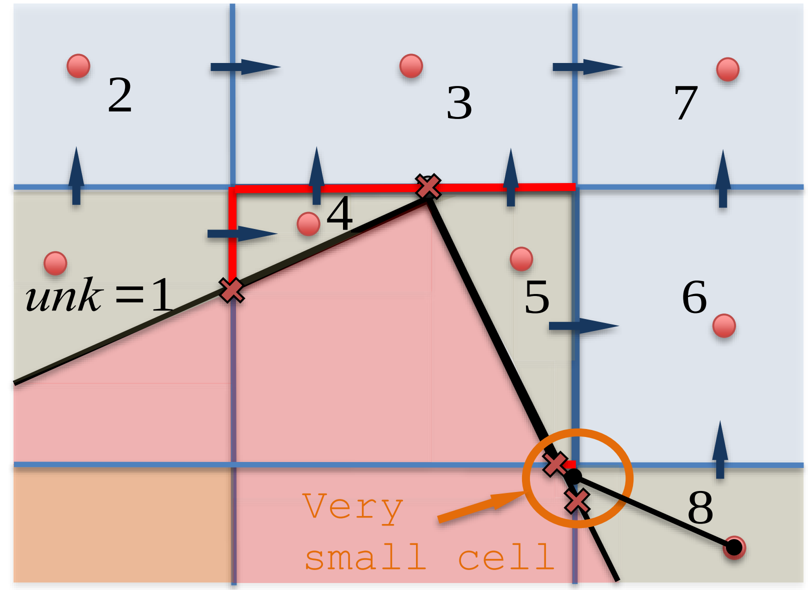
- S. May, M. Berger. Proc. Finite Vol. Cmplx App. VII, pp. 393-400 (2014).





Scalar Transport

- **Number** cell centered **unknowns** for $(rY_a)^{n+1}$.
- Build **face lists** on implicit region (cut-face and regular, GASPHASE or INBOUNDARY).
- Advection diffusion **matrices are built** by face. End result in CSR format.
- The corresponding discretized matrix-vector system:



Implicit (BE):

$$\left[\mathbf{M} + \mathrm{D}t\left(\mathbf{A}_{adv} + \mathbf{A}_{diff}\right)\right]\{rY_a\}^{n+1} = \mathbf{M}\{rY_a\}^{n} + \mathrm{D}t\{f\}$$

- Implicit: Solve using the **Intel MKL Pardiso**. Explicit: Trivial as **M** is diagonal.
- Very small cells cause **ill conditioned** systems. **Link** small cells to neighbors when $Vol_{CC} < C_{link} Vol_{Cart}$ and C_{link} » 10^{-4}.
- Fully explicit option (FE): $[\mathbf{M}]\{rY_a\}^{n+1} = \left[\mathbf{M} - \mathrm{D}t\left(\mathbf{A}_{adv} + \mathbf{A}_{diff}\right)\right]\{rY_a\}^{n} + \mathrm{D}t\{f\}$ $\quad C_{link}$ » 0.95

Energy

We factor the velocity divergence from the sensible enthalpy evolution equation (FDS).

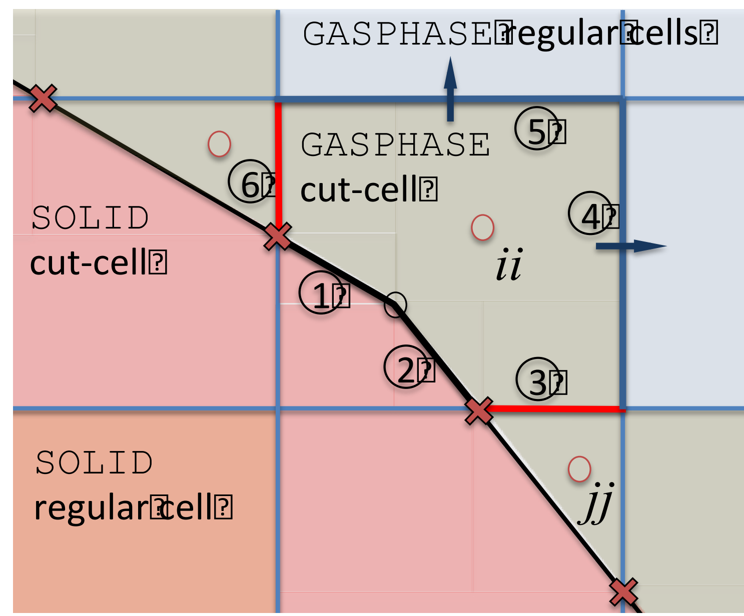
Objective:

- Discretize terms in thermodynamic divergence consistently with the scalar transport formulation for cut-cells (unstructured finite volume mesh).
- Use divergence integral equivalence to relate this divergence to the FDS Cartesian mesh.

Our Scheme:

- Implemented transport terms in cut-cells.
- Added combustion in regular cells of cut-cell region, radiation next.
- Linked cells for scalar transport get volume averaged thermodynamic divergence.

$$
\begin{aligned}
(\nabla\cdot\mathbf{u})^{th}_{ii}\,V_{ii} \;=\;& \left[\frac{1}{(\rho c_p T)_{ii}}-\frac{1}{\bar{p}_{ii}}\right]\frac{\partial \bar{p}_{ii}}{\partial t}\,V_{ii}+\frac{w_{ii}\,\rho_0 g_z}{(\rho c_p T)_{ii}} \\
&+\;\frac{1}{(\rho c_p T)_{ii}}\left[\dot{q}'''V_{ii}-\sum_{k=1}^{nf_c}\dot{\mathbf{q}}''_{ii,k}\cdot\hat{\mathbf{n}}_{ii,k}A_k-\overline{\mathbf{u}\cdot\nabla(\rho h_s)}V_{ii}\right] \\
&+\;\frac{1}{\rho_{ii}}\sum_{\alpha}\left(\frac{\overline{W}}{W_\alpha}-\frac{h_{s,\alpha}}{c_pT}\right)_{ii}\left[\dot{m}'''_\alpha V_{ii}-\sum_{k=1}^{nf_c}\mathbf{J}_{\alpha,ii,k}\cdot\hat{\mathbf{n}}_{ii,k}A_k-\overline{\mathbf{u}\cdot\nabla(\rho Y_\alpha)}V_{ii}\right]
\end{aligned}
$$



Schematic of cut-cell in 2D: velocities and fluxes on faces, and scalars defined in cells.

Momentum Coupling

Scheme sequence:

1. Time advancement of scalars on cut-cells and regular gas cells.

2. IBM Interpolation to get **target velocities** in cut-faces

$$u_i^{ibm} = c_0 u_i^B + c_1 u_i^{\text{int}}$$

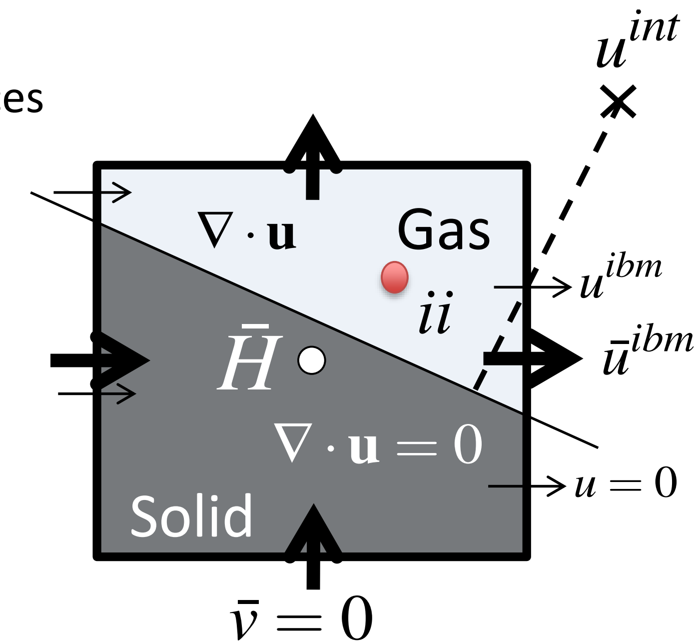
1. Flux **average** target velocities to Cartesian faces.

$$\bar{u}_i^{ibm} = \frac{1}{A_{cart}} \sum_k (u_i^{ibm} A_{cf})_k$$

1. Compute **direct forcing at Cartesian level**:

$$\bar{F}_i^n = -\left(\frac{\bar{u}_i^{ibm} - \bar{u}_i^n}{\Delta t} + \frac{\delta \bar{H}^n}{\delta x_i} \right)$$

1. Compute **thermodynamic divergence** on $(\nabla \cdot \mathbf{u})_{ii}^{th}$ cut-cells.



Momentum Coupling

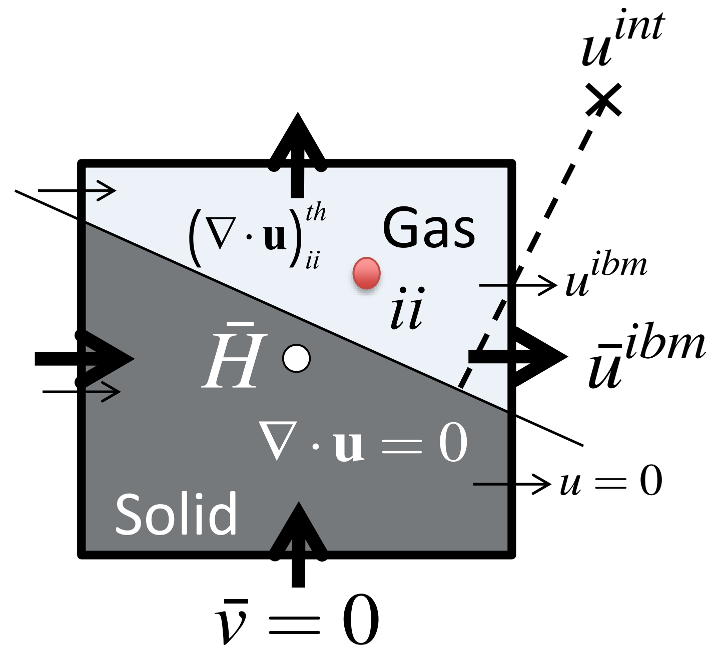
6. Use ***divergence integral equivalence***

$$\int_{\Omega_{cart}} (\nabla \cdot \bar{\mathbf{u}})^{th} d\Omega = \sum_{ii} \int_{\Omega_{ii}} (\nabla \cdot \mathbf{u})^{th}_{ii} d\Omega$$

to get Cartesian level target divergence $(\nabla \cdot \bar{\mathbf{u}})^{th}$.

7. Solve Cartesian level Poisson equation

$$\nabla^2 \bar{H} = -\left(\nabla \cdot \bar{\mathbf{F}}^n + \frac{(\nabla \cdot \bar{\mathbf{u}})^{th} - (\nabla \cdot \bar{\mathbf{u}})^n}{\Delta t} \right)$$



(in order to avoid mass penetration into body, solve on gas phase and cut-cell underlying Cartesian cells).

8. Project Cartesian velocities into target divergence field $\bar{\mathbf{u}}^{n+1} = \bar{\mathbf{u}}^n - \Delta t \left(\bar{\mathbf{F}}^n + \nabla \bar{H} \right)$

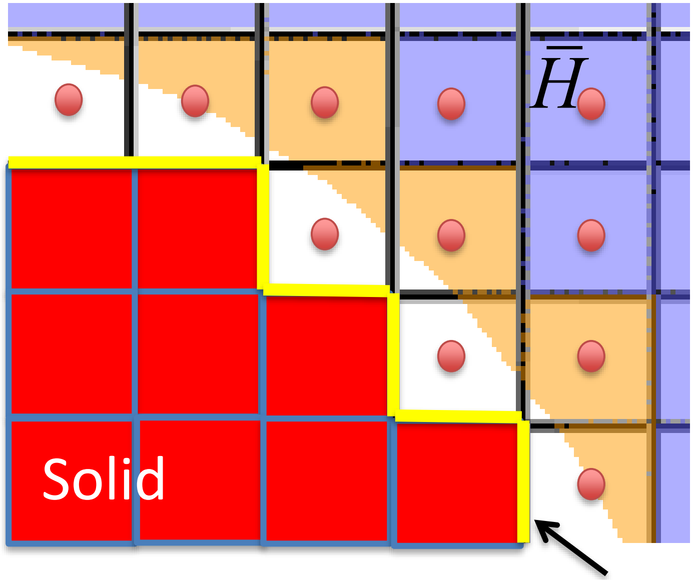
9. Reconstruct cut-face velocities.

Poisson Equation

- IBM: solve Poisson equation on the whole Cartesian domain, including cells within the immersed solids.
- Introduces mass penetration into the solid on the projection step. Undesirable for conservation, combustion.
- Our Momentum Coupling scheme: use this type of Pressure solver, or an **unstructured solution on Cartesian gas cells and cells underlying cut cells**.

Global linear system solver:

- Building a global Laplacian matrix in parallel.
- Building the global RHS.
- Calling Parallel Matrix-Vector solver, currently MKL **cluster sparse direct solver**.
- Capability to define correct H boundary condition in FDS &OBSTS and complex geometry bodies &GEOM.



$$\frac{\partial \bar{H}}{\partial x_n} = 0$$

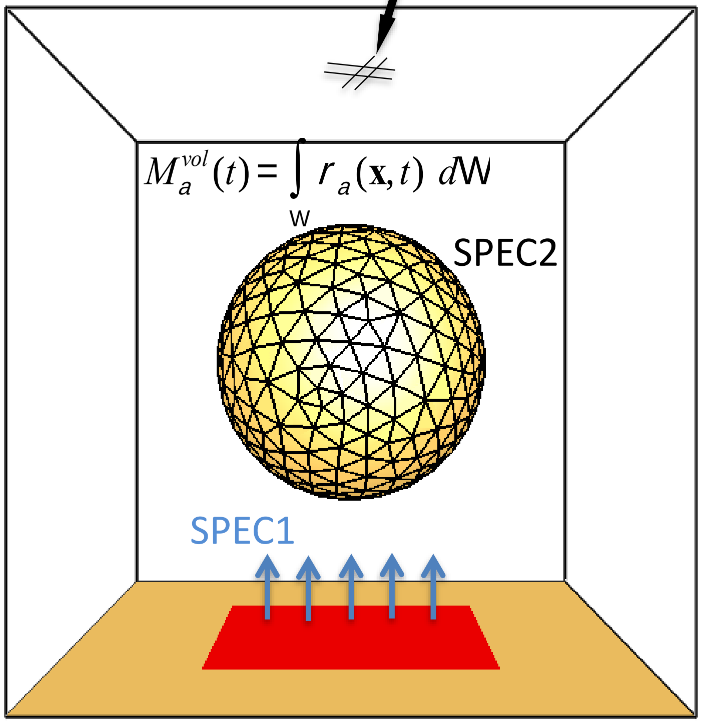
Example

- **Isothermal Gas Plume around immersed sphere:**

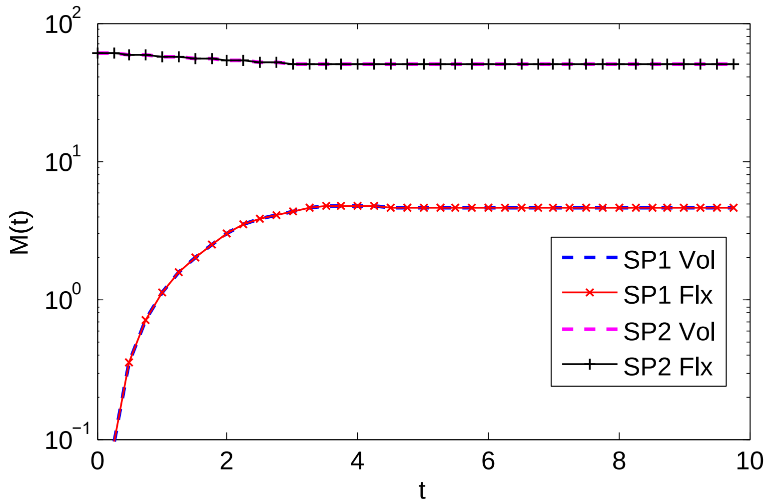
  Test conservation of EXIM scalar transport and transport terms in divergence expression for cut-cells.

- **Two species**: SPEC1: MW ~ 12, SPEC2: MW ~ 24 kg/mol.
- $m = 0.0005; \; D = 0.0002$ SI units.
- Inflow on bottom VENT, open boundary on others.
- Re=4000 based on unit velocity (inflow) and SPEC2 density.
- SPEC2 taken as background, DNS mode.
- Run for 10s, dt=0.0025, 40^3 Cartesian cells.
- Transport for **scalars** in cut-cell region using **BE Predictor + Trapezoidal Corrector**, solved with MKL **Pardiso**.
- **Poisson equation** defined in regular gas and cut-cell underlying Cartesian cells, solved with MKL **Pardiso**.
- Scalar calculation takes about twice the time of FDS using a square block OBST.
- Check total mass deficit of species as volume integral vs. domain boundary mass flux time integrals.

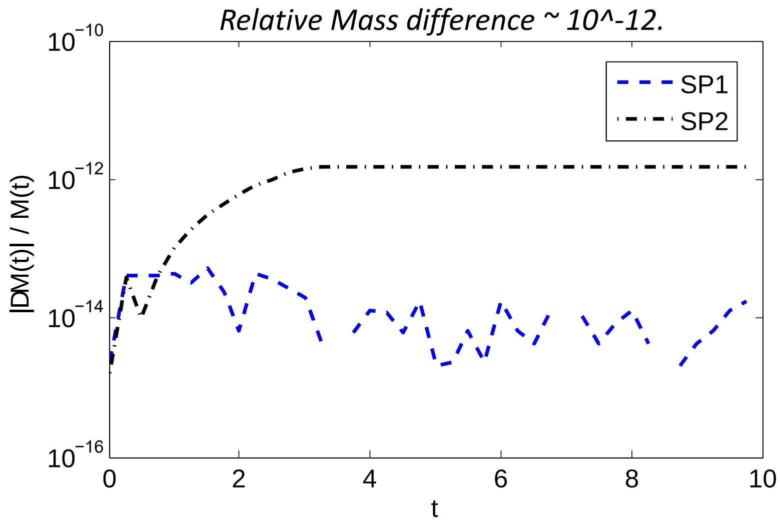
$$M_\alpha^{flx}(t) = M_\alpha^{vol}(t_0) + \int_{t_0}^{t} \int_{\Gamma} \dot{m}''_\alpha(\mathbf{x},t') \; d\Gamma dt'$$



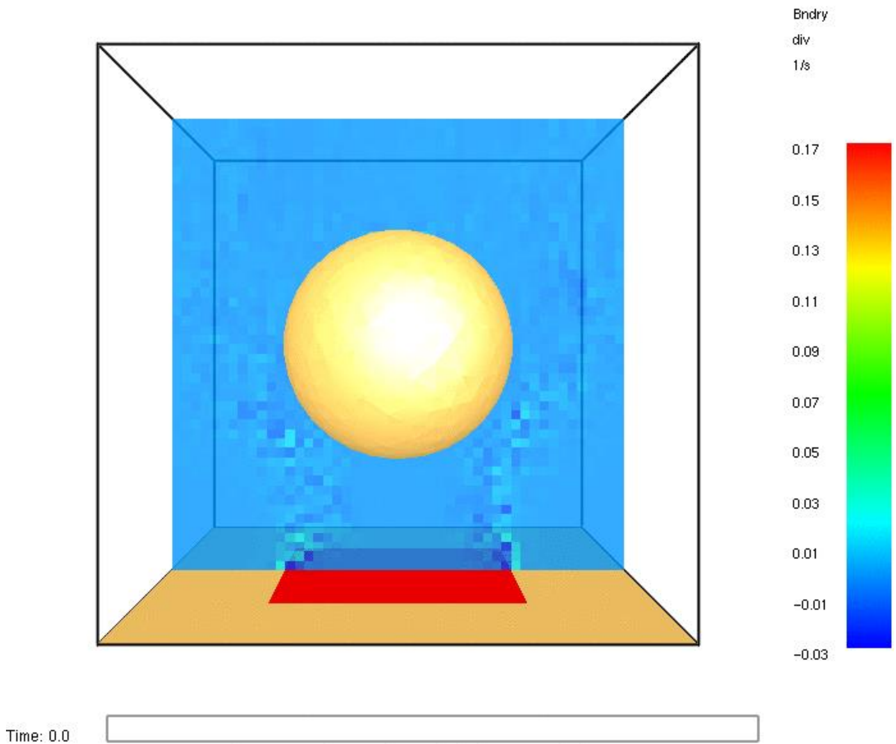
Example



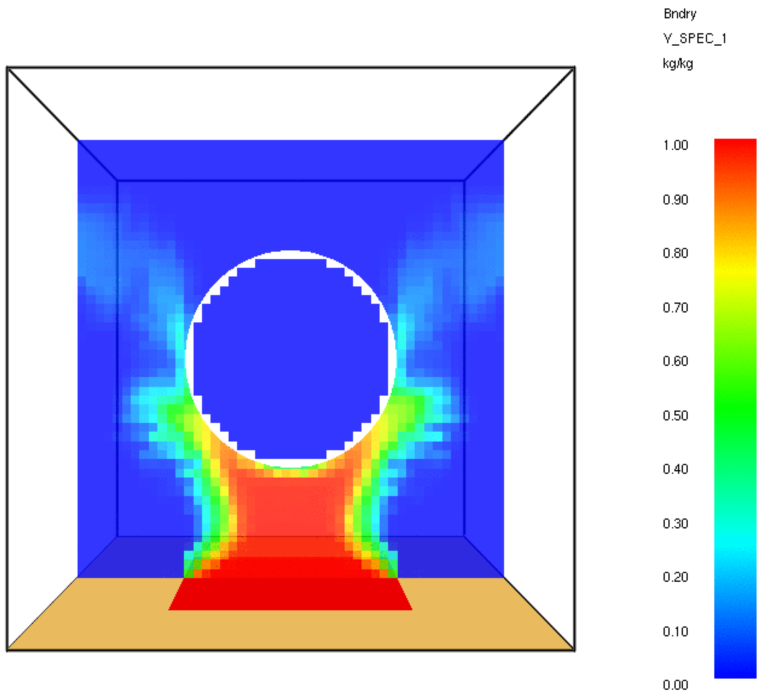
10^2
10^1
10^0
10^-1
M(t)
SP1 Vol
SP1 Flx
SP2 Vol
SP2 Flx
0
2
4
6
8
10
t



Relative Mass difference ~ 10^-12.
10^-10
10^-12
10^-14
10^-16
|DM(t)| / M(t)
SP1
SP2
0
2
4
6
8
10
t



Bndry
div
1/s
0.17
0.15
0.13
0.11
0.09
0.07
0.05
0.03
0.01
−0.01
−0.03
Time: 0.0



Bndry
Y_SPEC_1
kg/kg
1.00
0.90
0.80
0.70
0.60
0.50
0.40
0.30
0.20
0.10
0.00

Example

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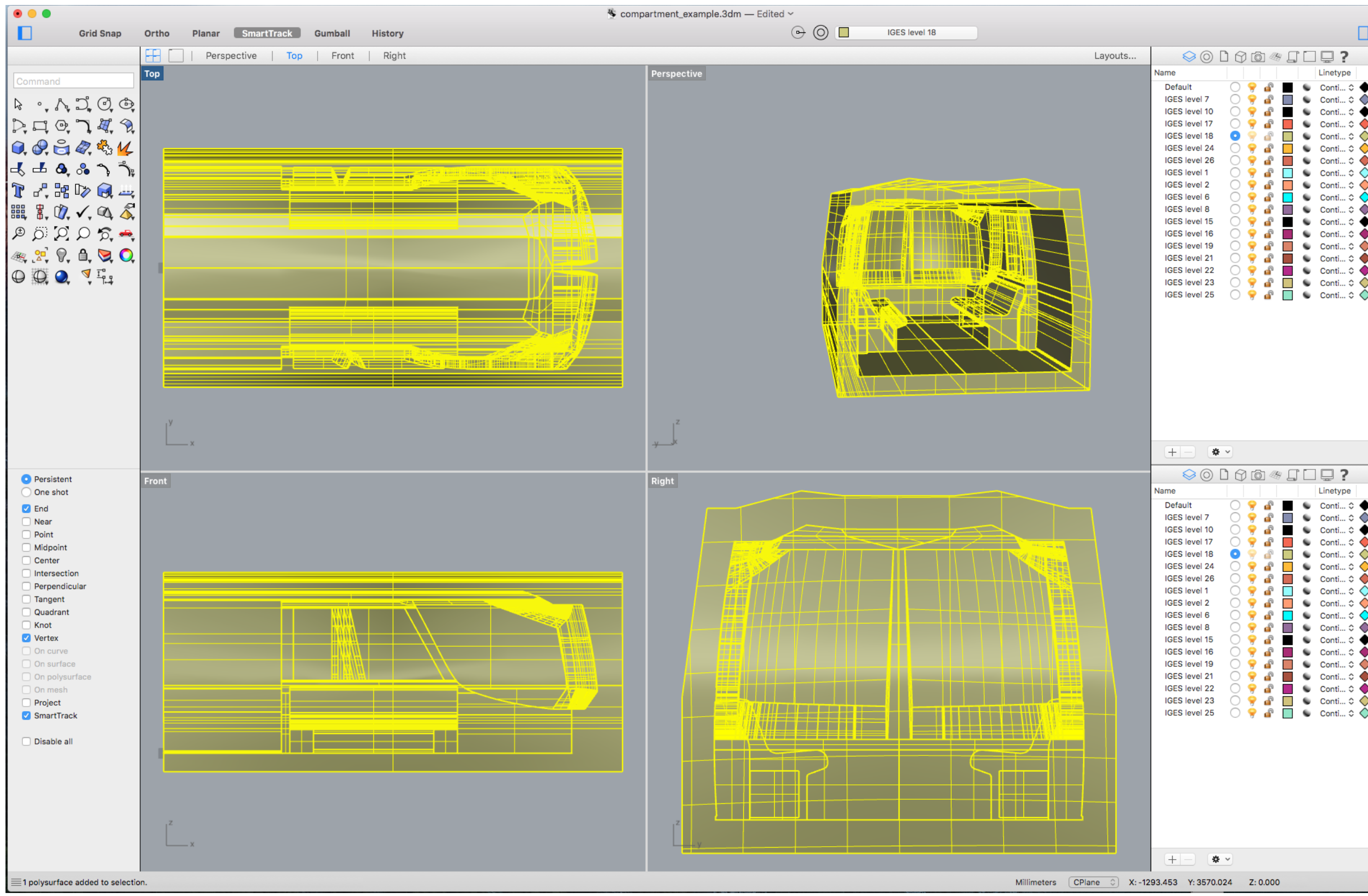
- **Propane fire in train cabin:**

FDS **&GEOM** definition Work flow

Realistic Train Cart model, courtesy of Fabian Braennstroem (Bombardier).

1. *Model defined in CAD software as a set of sanitized, disjoint volumes.*

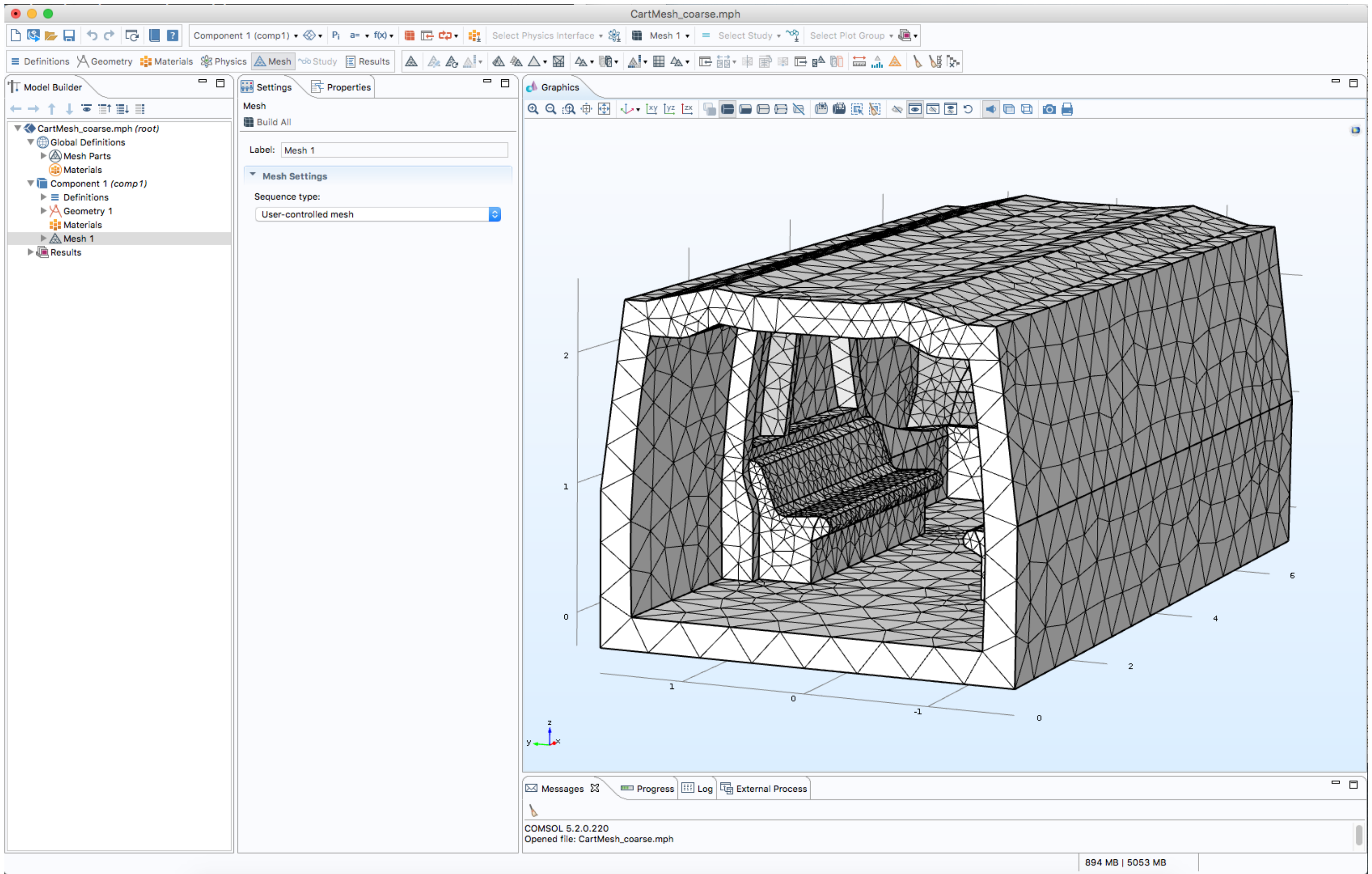
1. *Exported in format to read on meshing software (*.igs, *.stl).*



Example

3. *Geometry meshed in meshing software (i.e. COMSOL, Hypermesh, Gambit).*

4. *Mesh exported in neutral text format.*



Example

3. *Mesh file is converted into FDS input format.*

4. *Rest of simulation data is defined.*

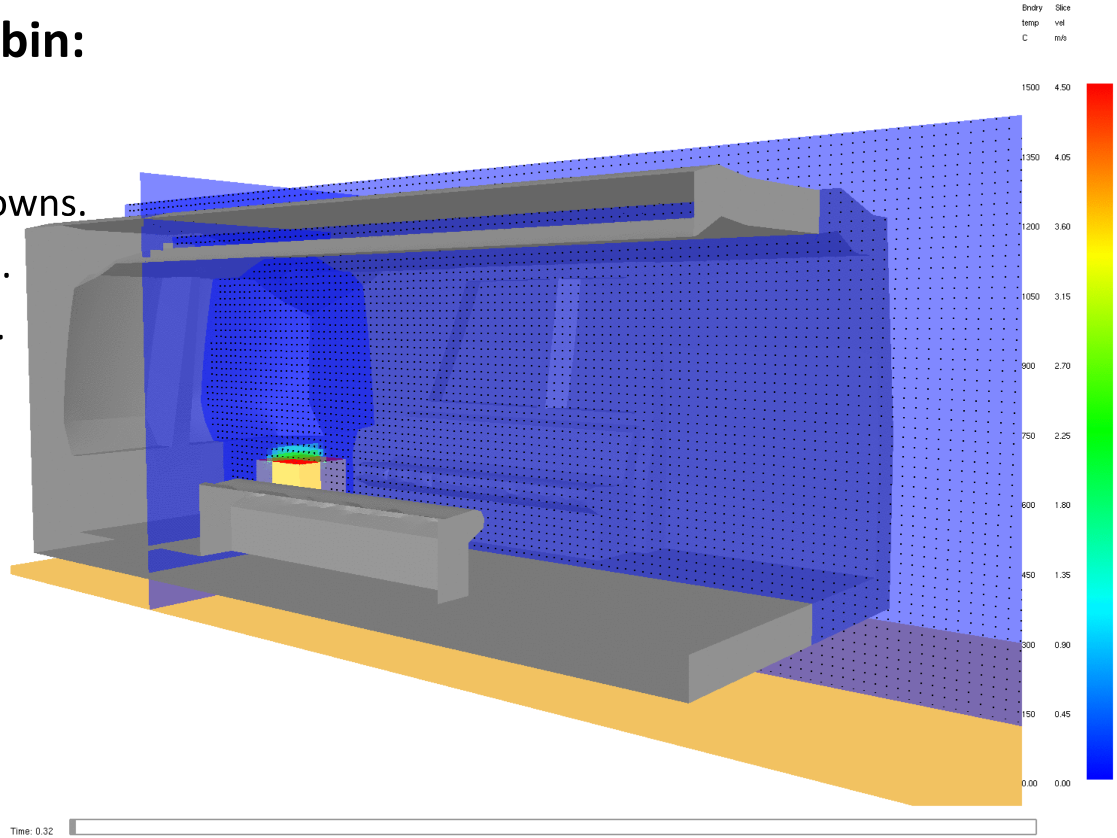
```
&HEAD CHID='cart_fire_800KW', TITLE='CC-IBM: Test propane fire on realistic train cart geometry.' /

&MESH IJK=144,78,58, XB=-2.75,7.25,-2.25,2.25,-0.5,2.85 /

&TIME T_END=50.0 /
&MISC DNS=.FALSE.,
      NOISE=.FALSE.
      STRATIFICATION=.FALSE.,
      CONSTANT_SPECIFIC_HEAT_RATIO=.FALSE.,
      BAROCLINIC=.FALSE.,
      PROJECTION=.TRUE.,
      CFL_VELOCITY_NORM=1,
      CC_IBM=.TRUE.,
      DO_IMPLICIT_CCREGION=.FALSE. /

&PRES GLMAT_SOLVER=.TRUE. /
&RADI RADIATION=.FALSE. /

# Vents:
&VENT MB='ZMAX', SURF_ID='OPEN' /
&VENT MB='YMIN', SURF_ID='OPEN' /
&VENT MB='YMAX', SURF_ID='OPEN' /
&VENT MB='XMIN', SURF_ID='OPEN' /
&VENT MB='XMAX', SURF_ID='OPEN' /

# Species:
&REAC FUEL='PROPANE', SOOT_YIELD=0.02 /

&SURF ID='BURNER', HRRPUA=3200., COLOR='RED' /
&SURF ID='cart', COLOR='GRAY', MATL_ID='cart', THICKNESS=0.1/
&MATL ID='cart', DENSITY=1, CONDUCTIVITY=1, SPECIFIC_HEAT=1/

# Geometries:
&OBST XB=4.5,5.0,-.75,-0.25,0.05,0.55, SURF_IDS='BURNER','INERT','INERT' /
&GEOM ID='FEM_MESH', MATL_ID='cart', SURF_ID='cart'
VERTS=
-0.00019300,      -1.68766011,      0.14260193,
-0.00056374,      -1.68765986,      0.55683507,
 1.78482997,      -0.59141201,      0.52607399,
```

cart_fire_800KW.fds demo FDS input file.

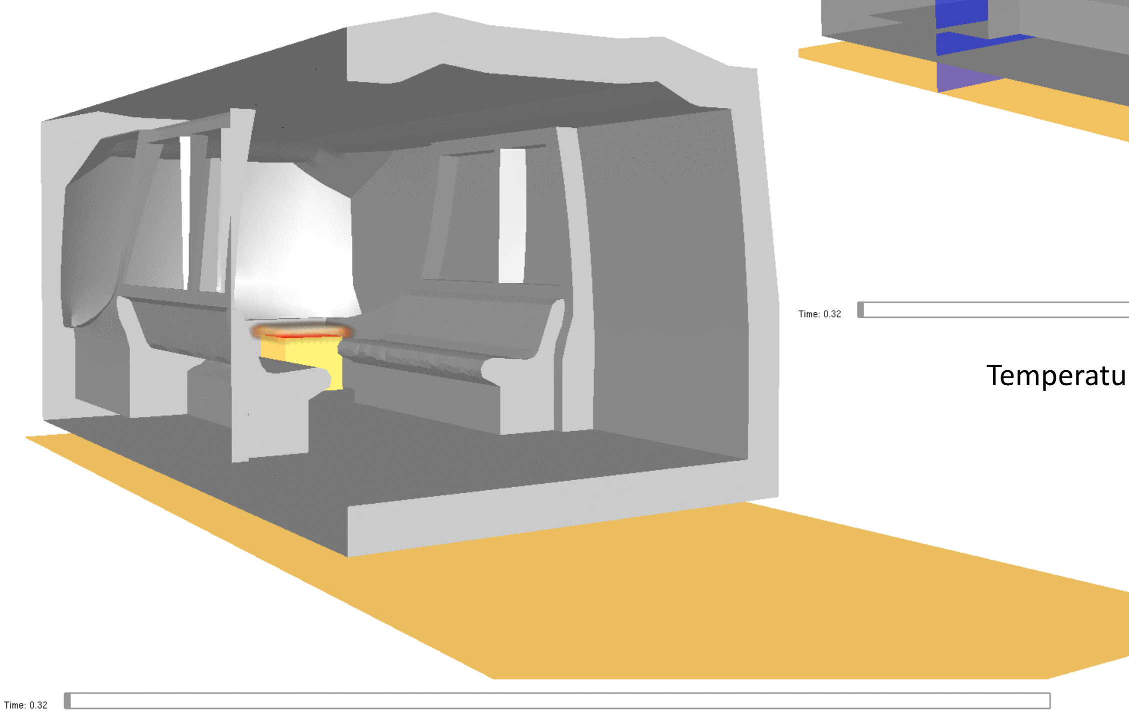
Example

- **LES of propane fire in train cabin:**

- 800 KW Propane burner.
- 144x78x58 grid, ~50K CC scalar unknowns.
- Explicit scalar integration in CC region.
- Unstructured Cartesian Poisson solve.



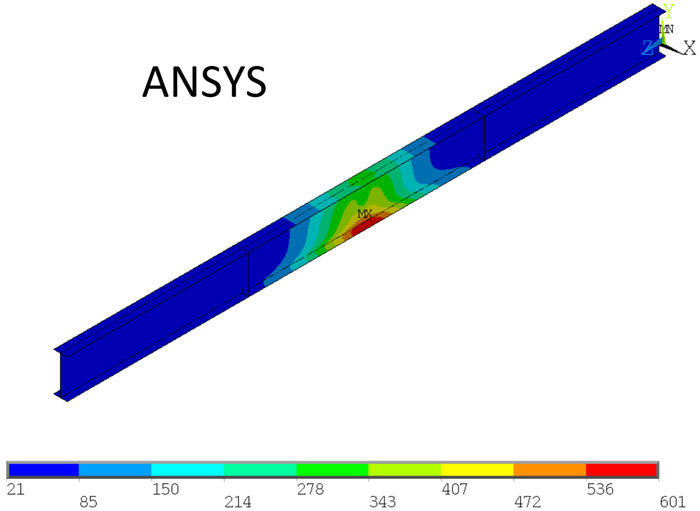
Temperature slice 20C (blue) to 1500C (red), + velocity vectors (black).

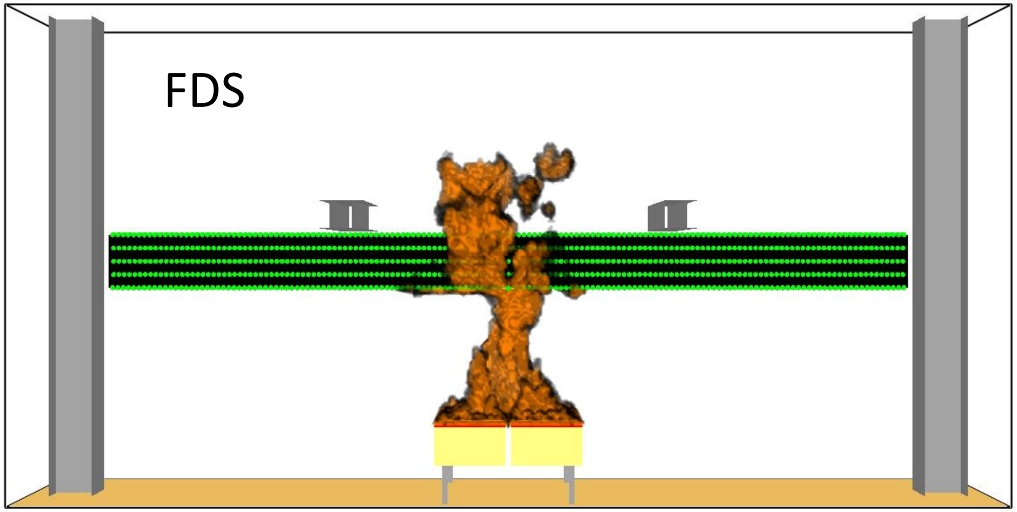


Smoke + HRRPUV contours.

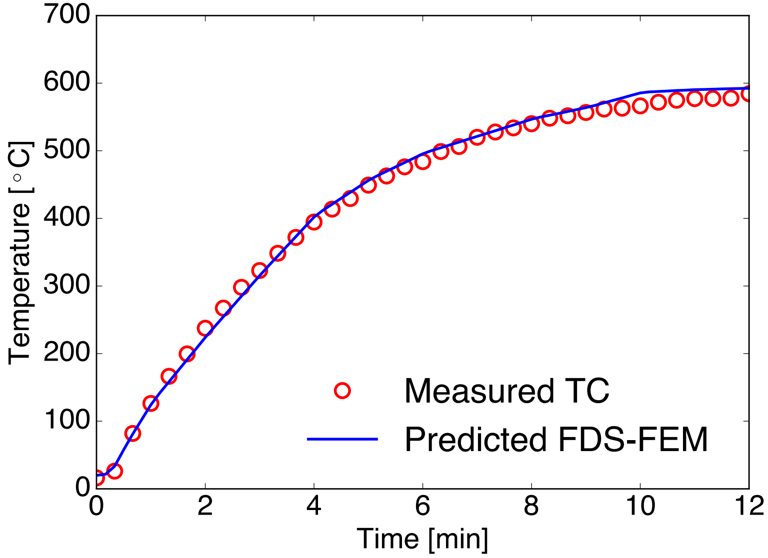
Future Work

- Verification and Validation.
- Enhance radiation solver to solve RTE on cut-cells, add radiative boundary conditions on boundary cut-faces.
- Extend the treatment of particles from Cartesian cells unstructured cut-cells.
- Develop the data transfer for two way coupling with thermo-mechanical FEM solvers + moving internal boundaries.





NFRL commissioning test, courtesy Chao Zhang.



Thank you