

Fire Dynamics Simulator: Advances on simulation capability for complex geometry

Marcos Vanella^{a,b}, Randall McDermott^b, Glenn Forney^b, Kevin McGrattan^b

^a*The George Washington University*

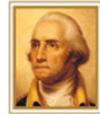
^b*National Institute of Standards and Technology*

Contents



- Motivation and Objective.
- 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



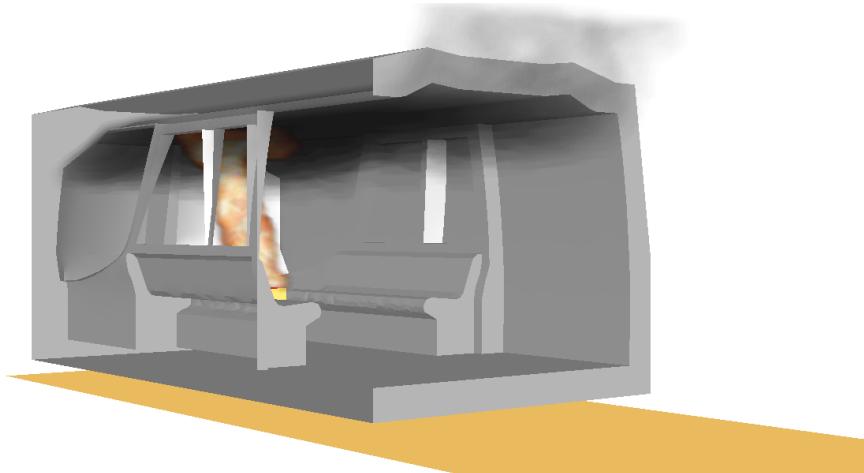
The Fire Dynamics Simulator* (FDS) is used in:

- 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.

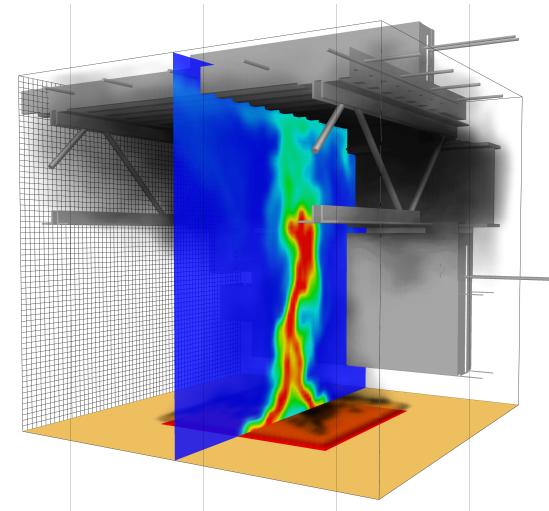
Objective:

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

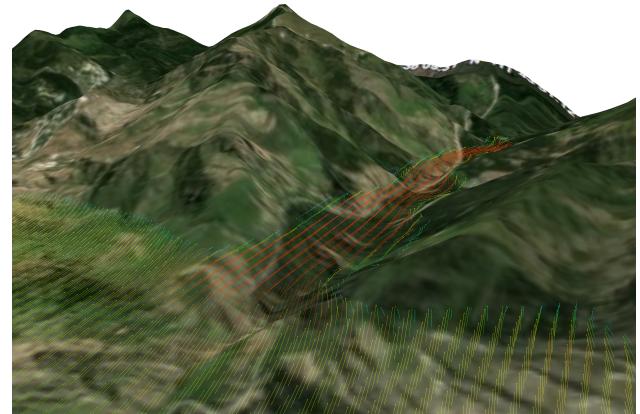


LES of 800 KW propane fire in open train cart. Geometry courtesy of Fabian Braennstroem (Bombardier).

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

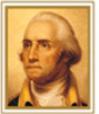


Fire-Structure Interaction: 12 MW fire load on a steel/concrete floor connection assembly.



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.

Motivation, Objective



Spatial discretization and time marching in FDS, work areas:

Scalar transport

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

EOS

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

Combustion, Radiation

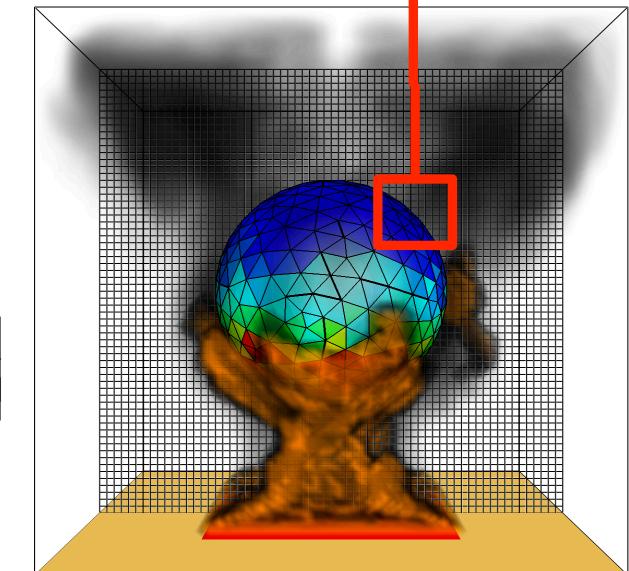
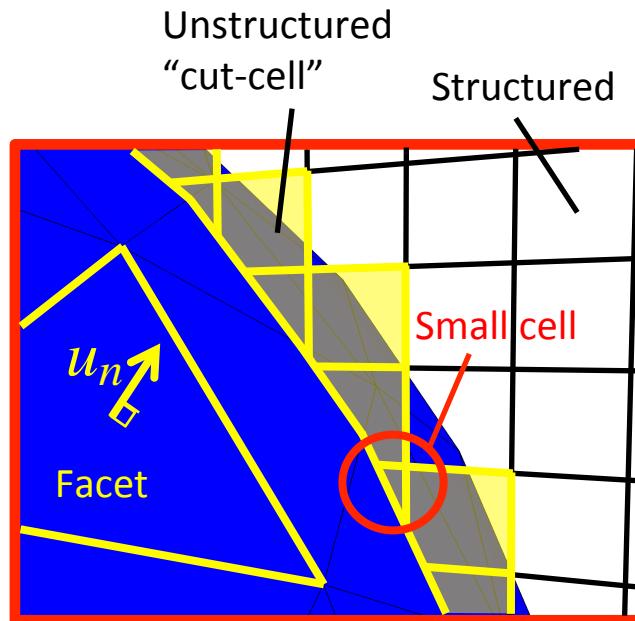
$$\left\{ \dot{\mathbf{q}}_R'' \quad \dot{\mathbf{q}}''' \right.$$

Divergence Constraint*

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

Momentum + IBM⁺

$$\left\{ \begin{aligned} \frac{\partial \mathbf{u}}{\partial t} &= -(\mathbf{F} + \nabla H^{n-1}) \rightarrow \mathbf{F}_{IB} = -\left(\frac{\partial \mathbf{u}}{\partial t} \right)_D - \nabla H^{n-1} \\ \frac{\partial}{\partial t} (\nabla \cdot \mathbf{u}) &\cong \frac{(\nabla \cdot \mathbf{u})^{n+1} - \nabla \cdot \mathbf{u}^n}{\Delta t}, \quad \Delta H = -\left[\nabla \cdot \mathbf{F} + \frac{\partial}{\partial t} (\nabla \cdot \mathbf{u}) \right] \\ \frac{\partial \mathbf{u}}{\partial t} &= -(\mathbf{F} + \nabla H) \end{aligned} \rightarrow \mathbf{u}^{n+1}, \Delta H^n \right.$$



* 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

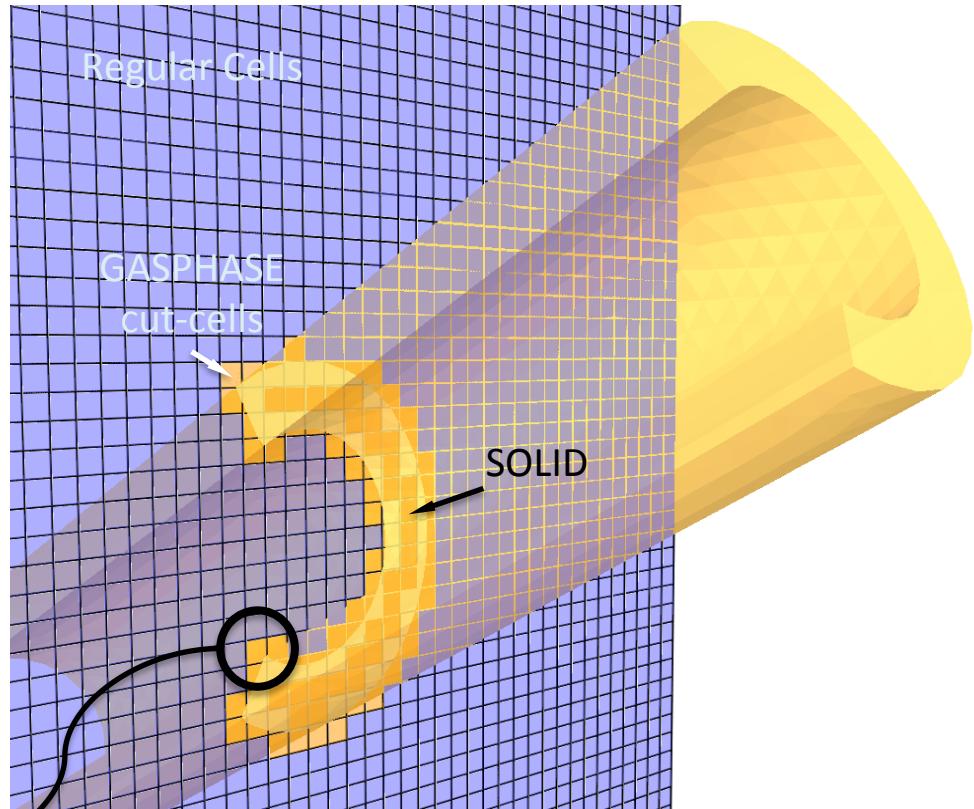
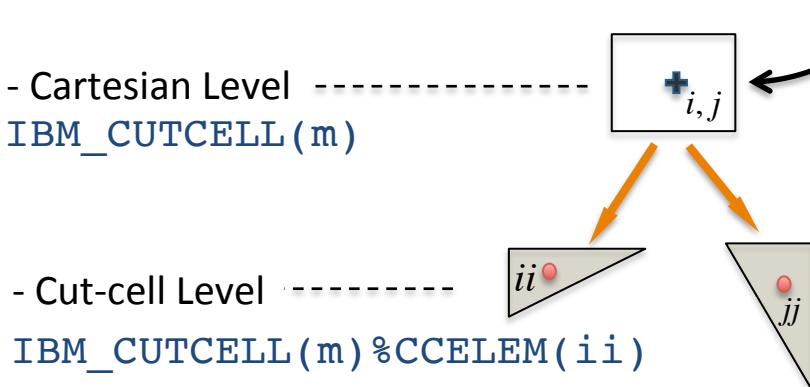


Objective:

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

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.



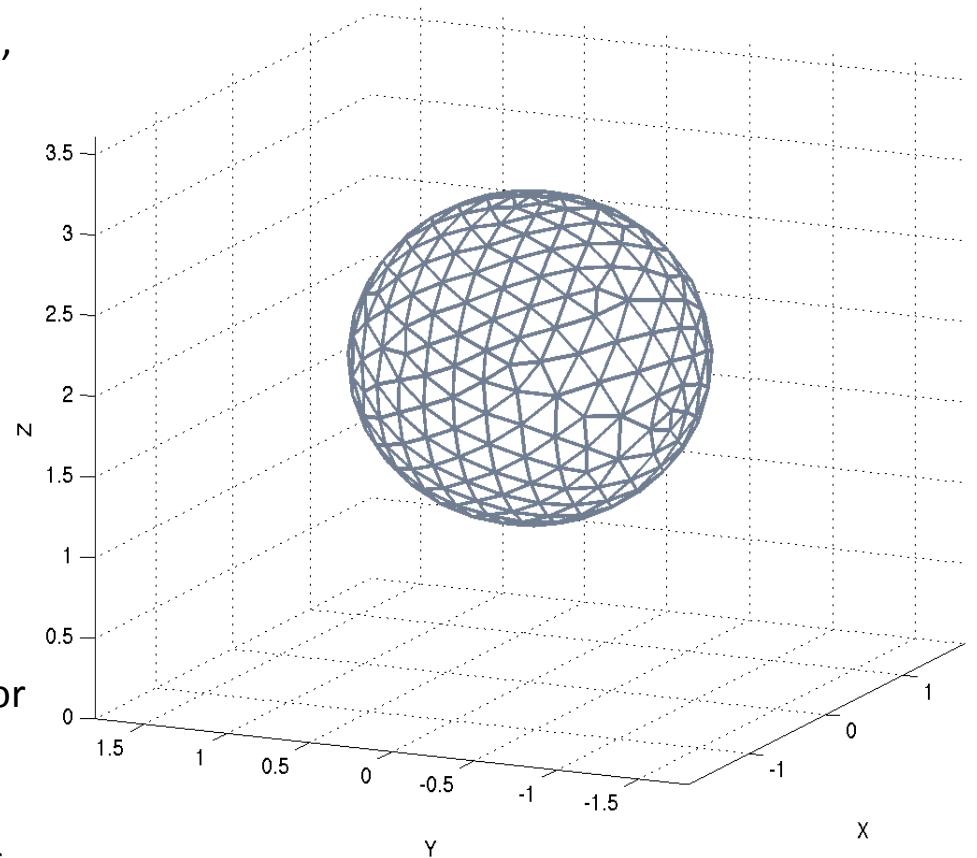
Smokeview Visualization inclined C-beam mid-plane. Obtained with computational geometry engine in FDS.

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: $\frac{\partial \rho Y_\alpha}{\partial t} + \nabla \cdot (\rho Y_\alpha \mathbf{u}) = -\nabla \cdot \mathbf{J}_\alpha + \dot{m}''_{\alpha} ; \quad \alpha = 1, \dots, N$ on domain + Ics, Bcs

Take: $\mathbf{J}_\alpha = -\rho D_\alpha \nabla Y_\alpha = -\left(D_\alpha \nabla(\rho Y_\alpha) - \frac{D_\alpha}{\rho} \nabla \rho (\rho Y_\alpha) \right)$

Then:

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

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

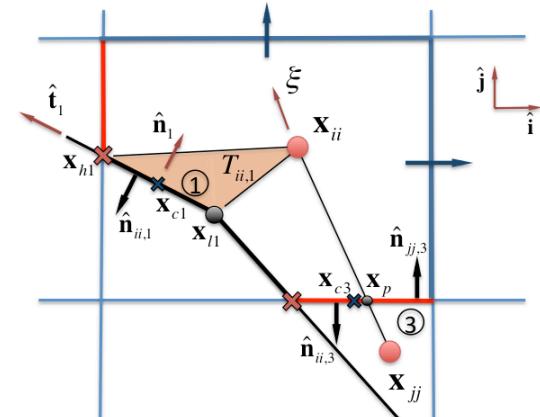
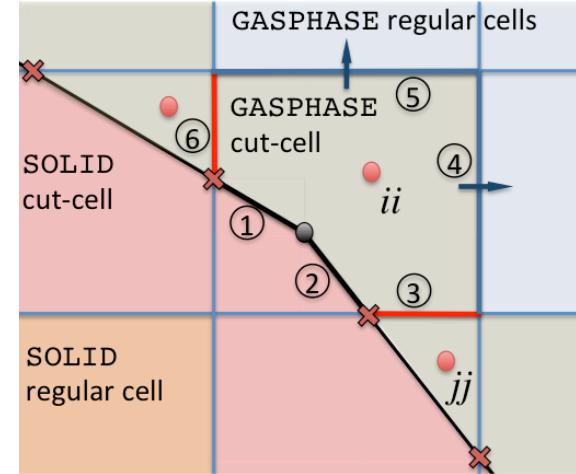
- **Advection:**

$$\int_{\Omega_{ii}} \nabla \cdot (\mathbf{u}' \rho Y_\alpha) d\Omega = \int_{\partial \Omega_{ii}} (\mathbf{u}' \rho Y_\alpha) \cdot \hat{\mathbf{n}}_{ii} d\partial \Omega = \sum_{k=1}^{nfc} (\mathbf{u}' \rho Y_\alpha)_k \cdot \hat{\mathbf{n}}_{ii,k} A_k$$

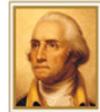
For a given face ($k=4$, cut-cell ii):

$$(\mathbf{u}' \rho Y_\alpha)_k \cdot \hat{\mathbf{n}}_{ii,k} A_k = \left[(\overline{\rho Y_\alpha})_k^{fl} \mathbf{u}_k + (\overline{\rho Y_\alpha})_k^{lin} \left(\frac{D_\alpha}{\rho} \nabla \rho \right)_k \right] \cdot \hat{\mathbf{n}}_{ii,k} A_k$$

- **Diffusion:** $\int_{\Omega_{ii}} \nabla \cdot (D_\alpha \nabla(\rho Y_\alpha)) d\Omega = \int_{\partial \Omega_{ii}} (D_\alpha \nabla(\rho Y_\alpha)) \cdot \hat{\mathbf{n}}_{ii} d\partial \Omega = \sum_{k=1}^{nfc} (D_\alpha \nabla(\rho Y_\alpha))_k \cdot \hat{\mathbf{n}}_{ii,k} A_k$



Scalar Transport

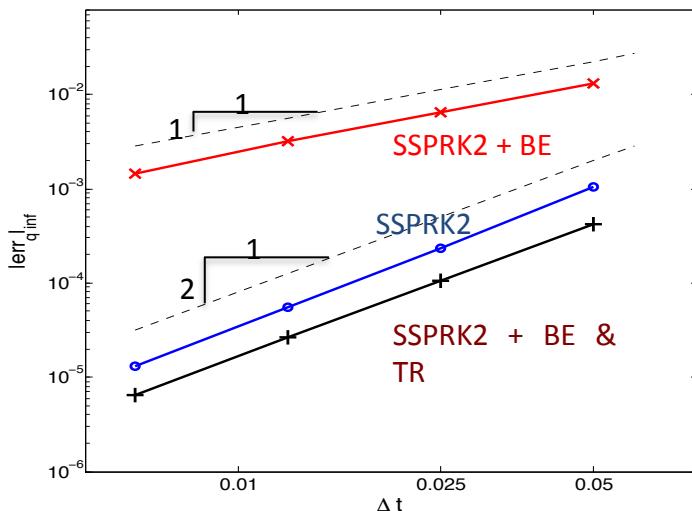
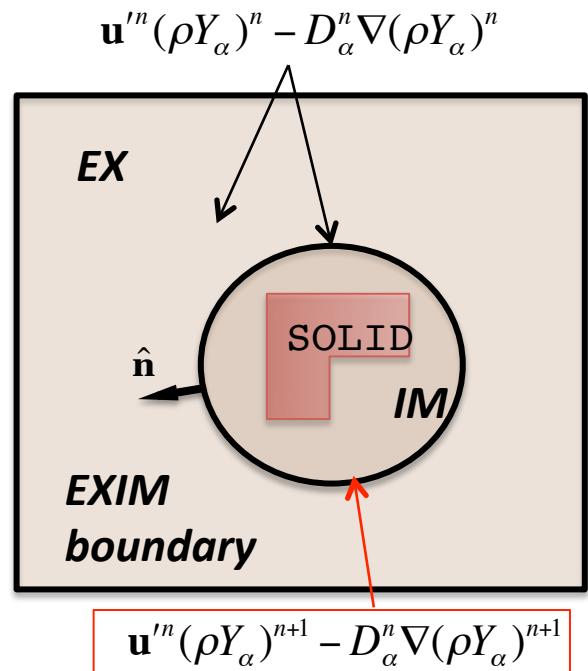


- Small cut-cells are problematic for explicit time integration.
- Alleviation methods tend to be arbitrary, deteriorating the solution quality.

Explicit - Implicit time integration*:

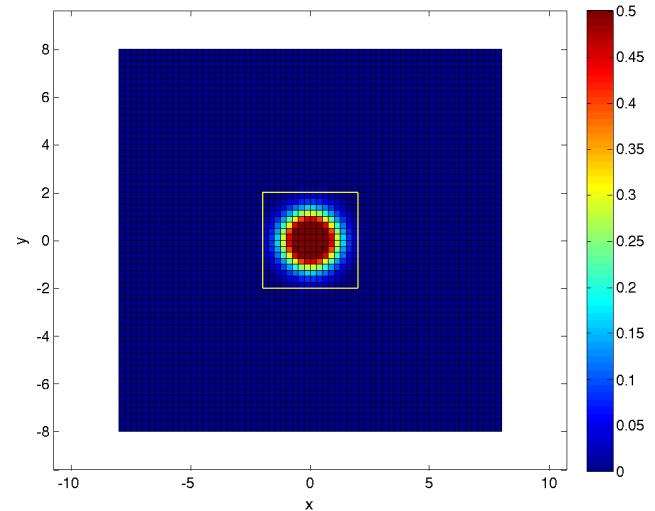
- **Explicit region:** Advance first.
- **Implicit region:** linearizing transport, i.e. implicit BE:

$$\frac{(\rho Y_\alpha)^{n+1} - (\rho Y_\alpha)^n}{\Delta t} = -\nabla \cdot (\boxed{\mathbf{u}'^n (\rho Y_\alpha)^n - D_\alpha^n \nabla (\rho Y_\alpha)^n})$$



*- 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).



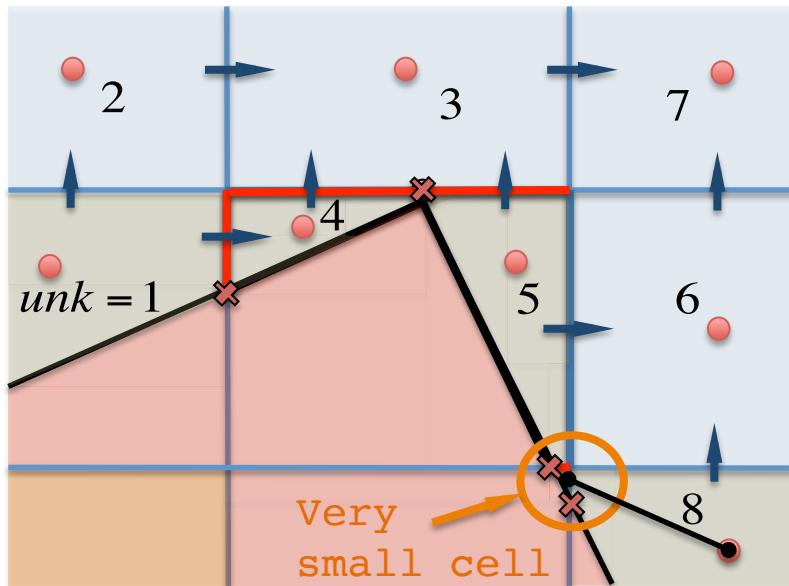
Scalar Transport



- Number cell centered **unknowns** for $(\rho Y_\alpha)^{n+1}$.
- 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):

$$[\mathbf{M} + \Delta t (\mathbf{A}_{adv} + \mathbf{A}_{diff})] \{\rho Y_\alpha\}^{n+1} = \mathbf{M} \{\rho Y_\alpha\}^n + \Delta t \{f\}$$



- 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 $C_{link} \approx 10^{-4}$.
- Fully explicit option (FE): $[\mathbf{M}] \{\rho Y_\alpha\}^{n+1} = [\mathbf{M} - \Delta t (\mathbf{A}_{adv} + \mathbf{A}_{diff})] \{\rho Y_\alpha\}^n + \Delta t \{f\}$ $C_{link} \approx 0.95$

Energy



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

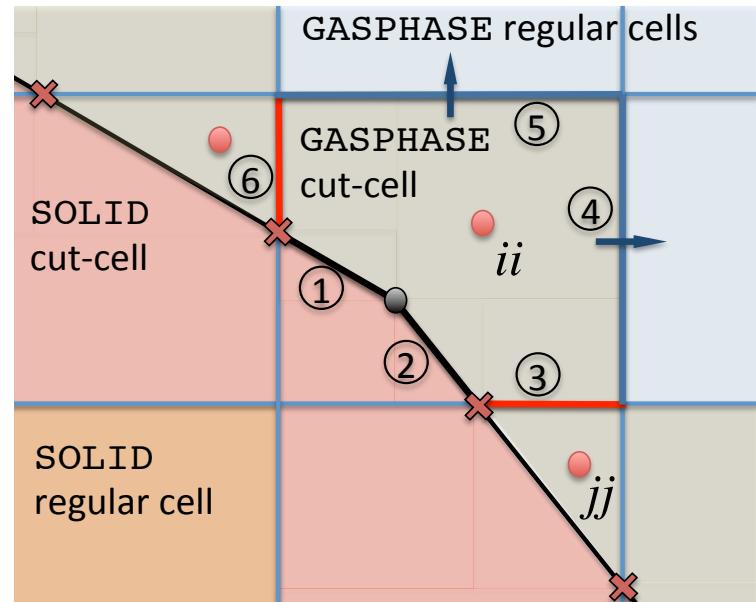
Objective:

- 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.

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



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

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

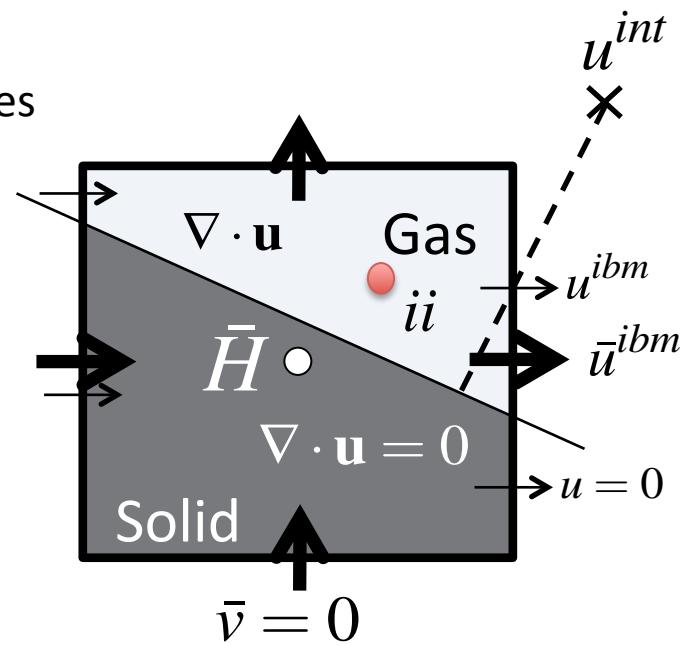
3. Flux **average** target velocities to Cartesian faces.

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

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

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

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



Momentum Coupling



6. Use *divergence integral equivalence*

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

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

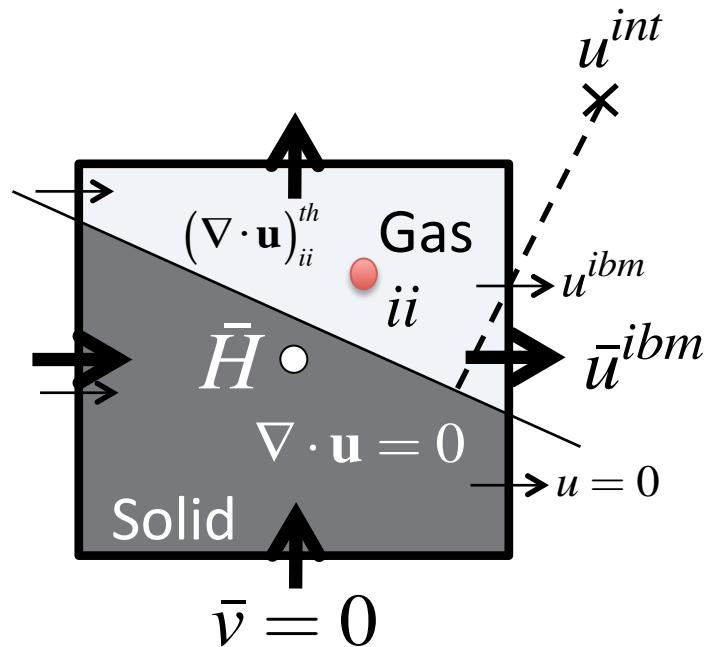
7. Solve Cartesian level Poisson equation

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

(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 $\bar{\mathbf{u}}^{n+1} = \bar{\mathbf{u}}^n - \Delta t (\bar{\mathbf{F}}^n + \nabla \bar{H})$

9. Reconstruct cut-face velocities.



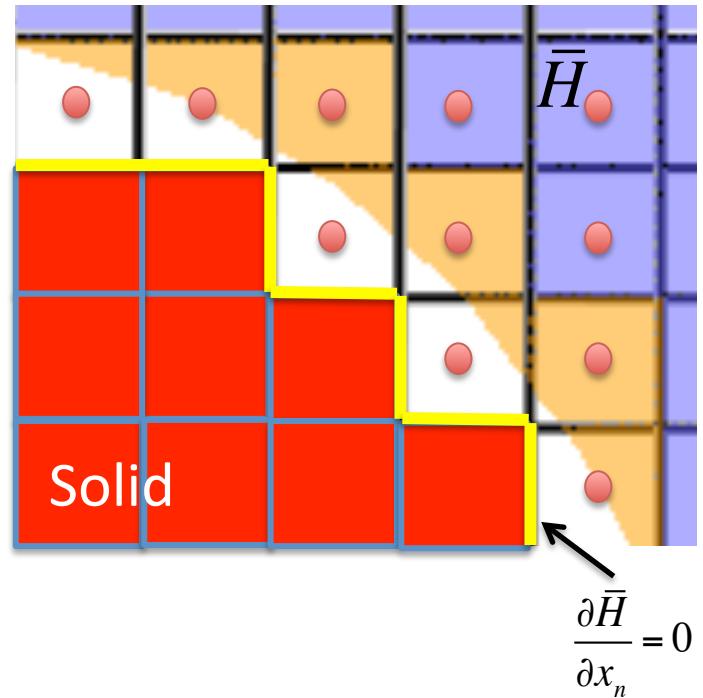
Poisson Equation



- 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.



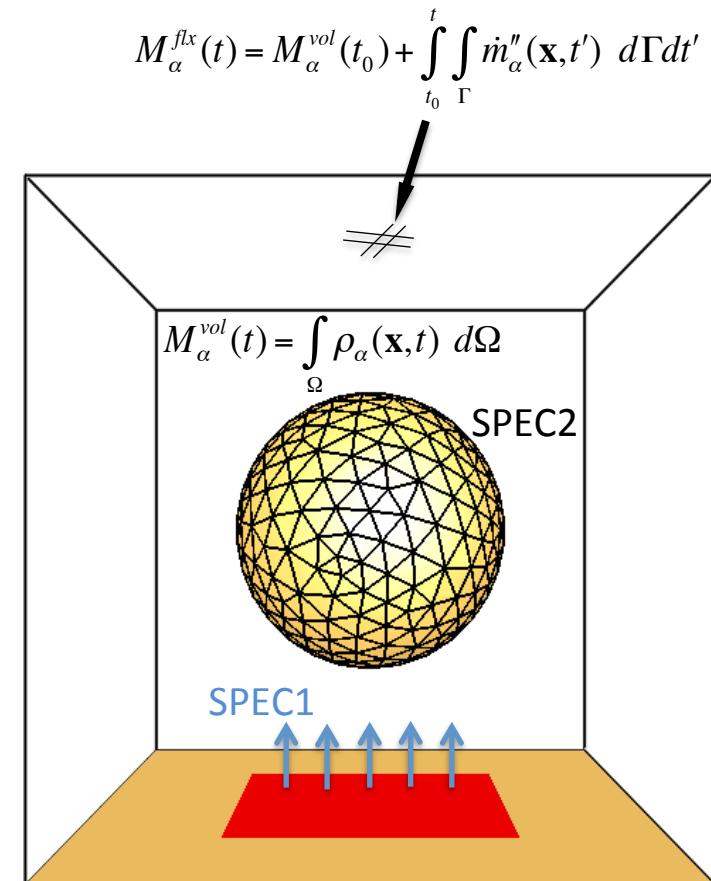
Example



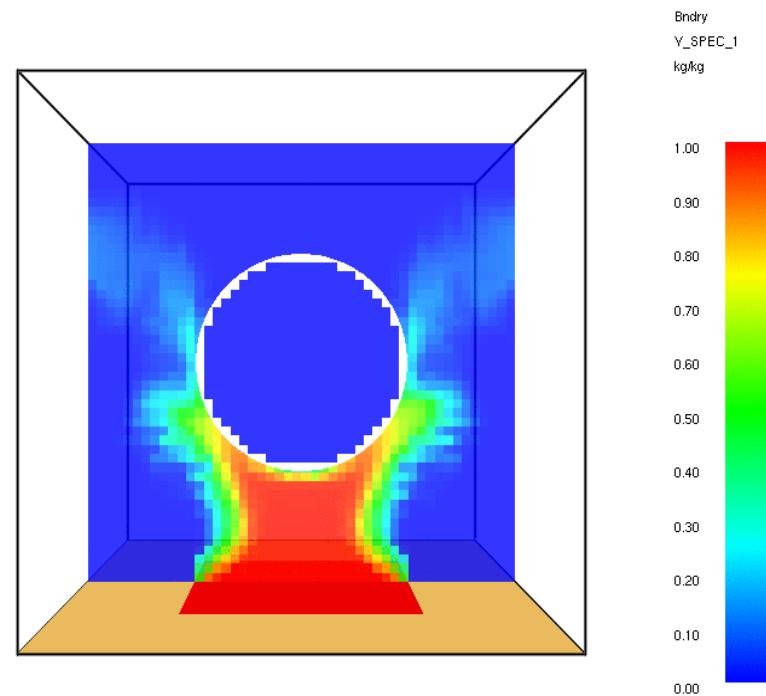
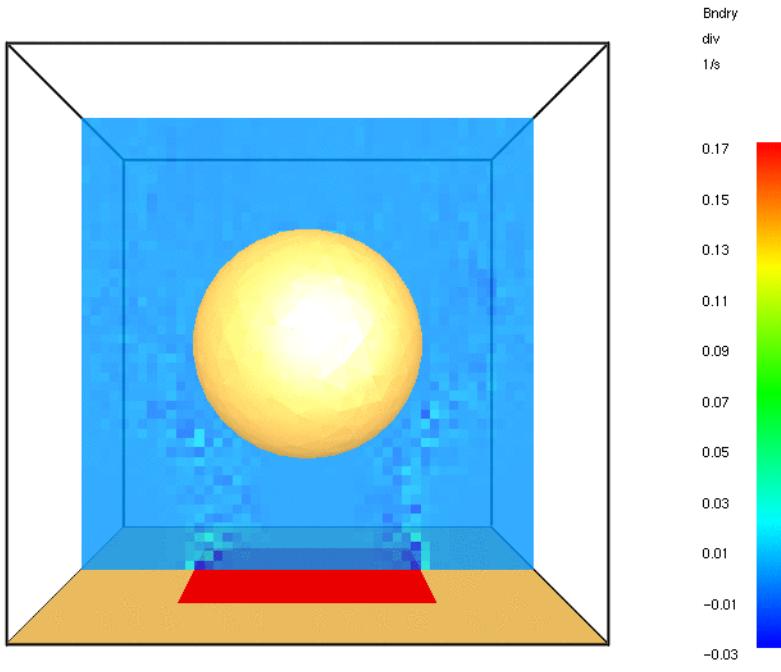
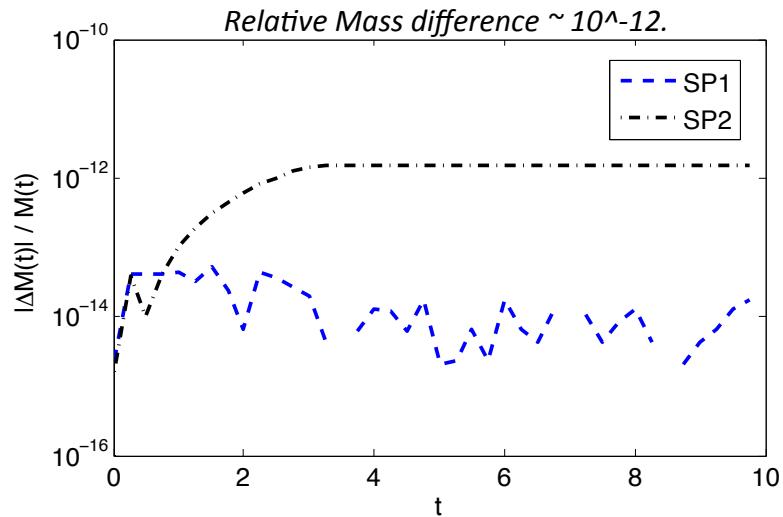
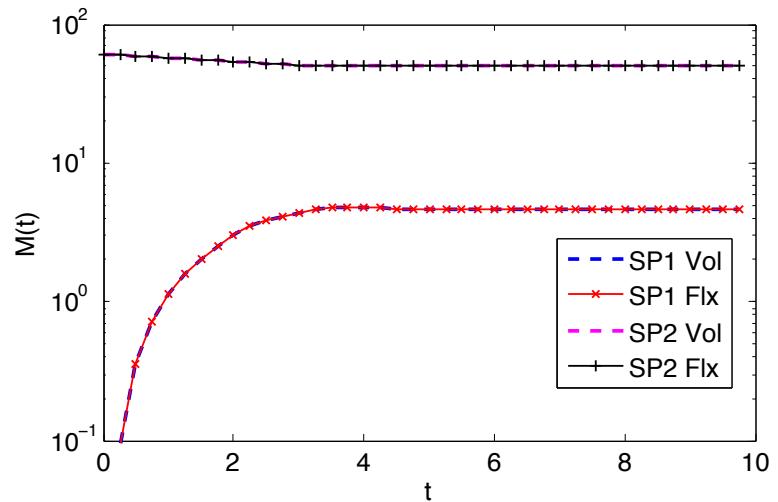
- **Isothermal Gas Plume around immersed sphere:**

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.
- $\mu = 0.0005$; $D = 0.0002$ 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.



Example



Example



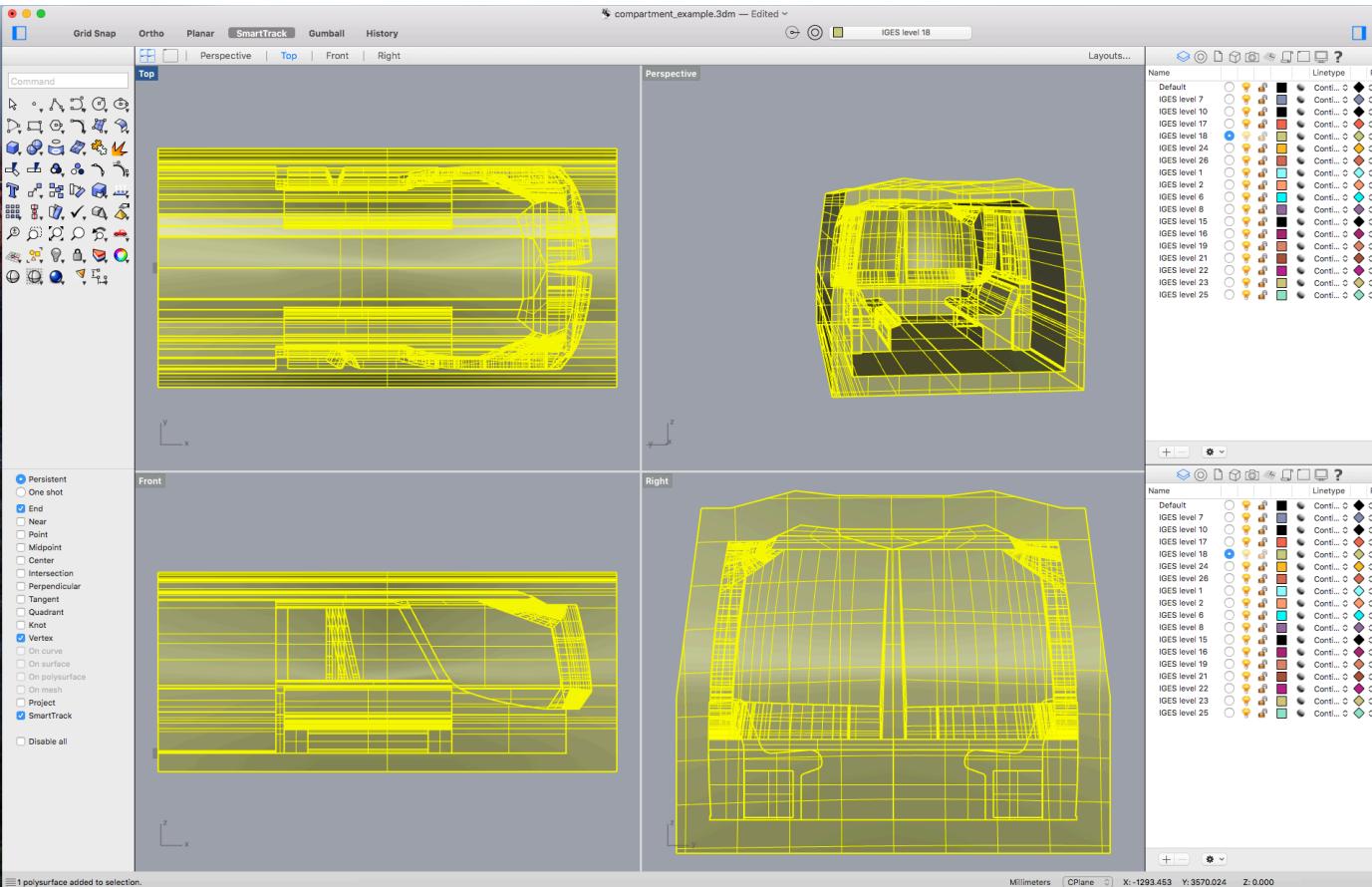
- **Propane fire in train cabin:**

FDS &GEOM definition Work flow

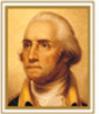
Realistic Train Cart model, courtesy of Fabian Braennstroem (Bombardier).

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

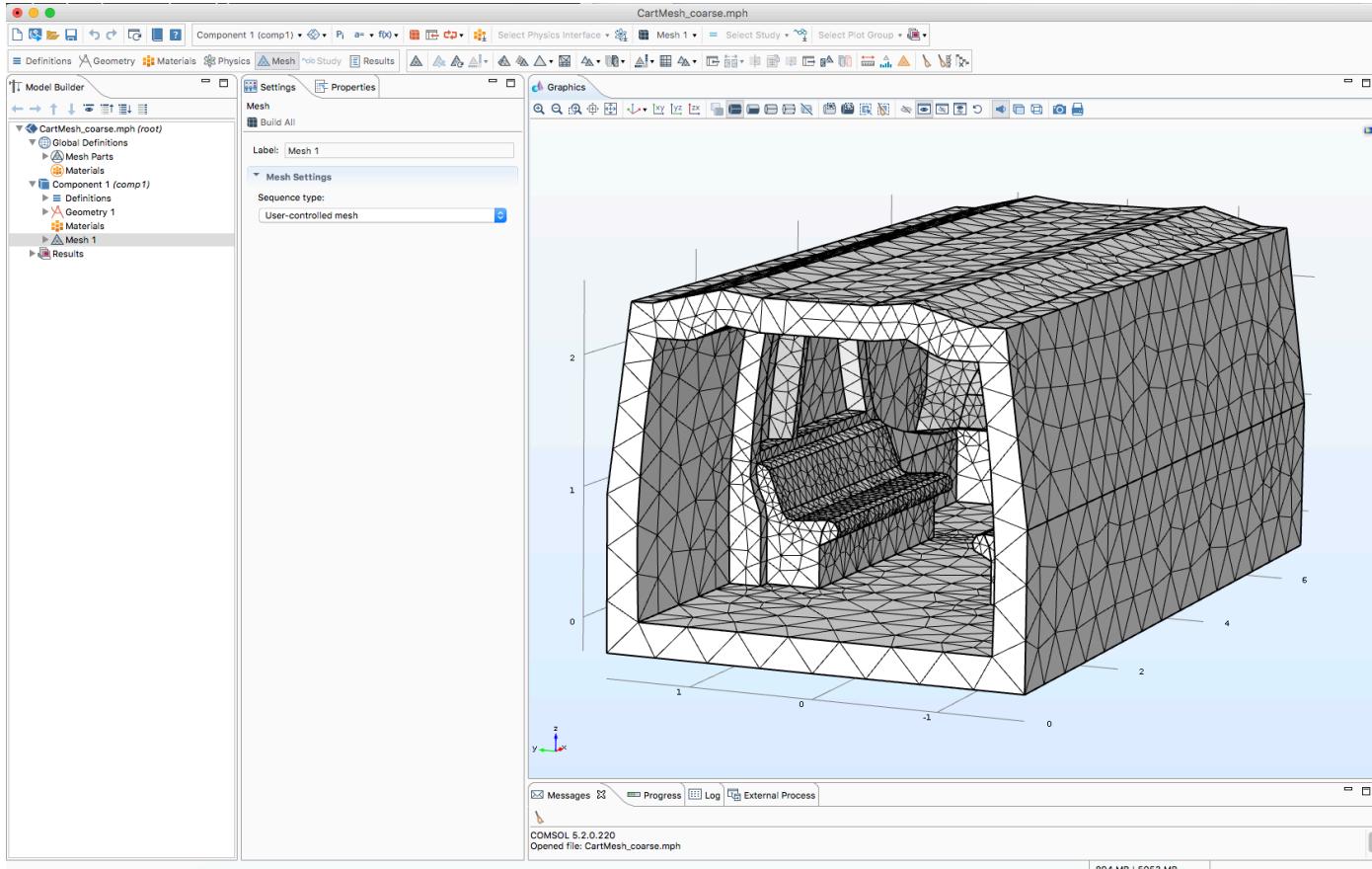
2. Exported in format to read on meshing software (*.igs, *.stl).



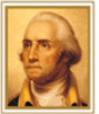
Example



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.*

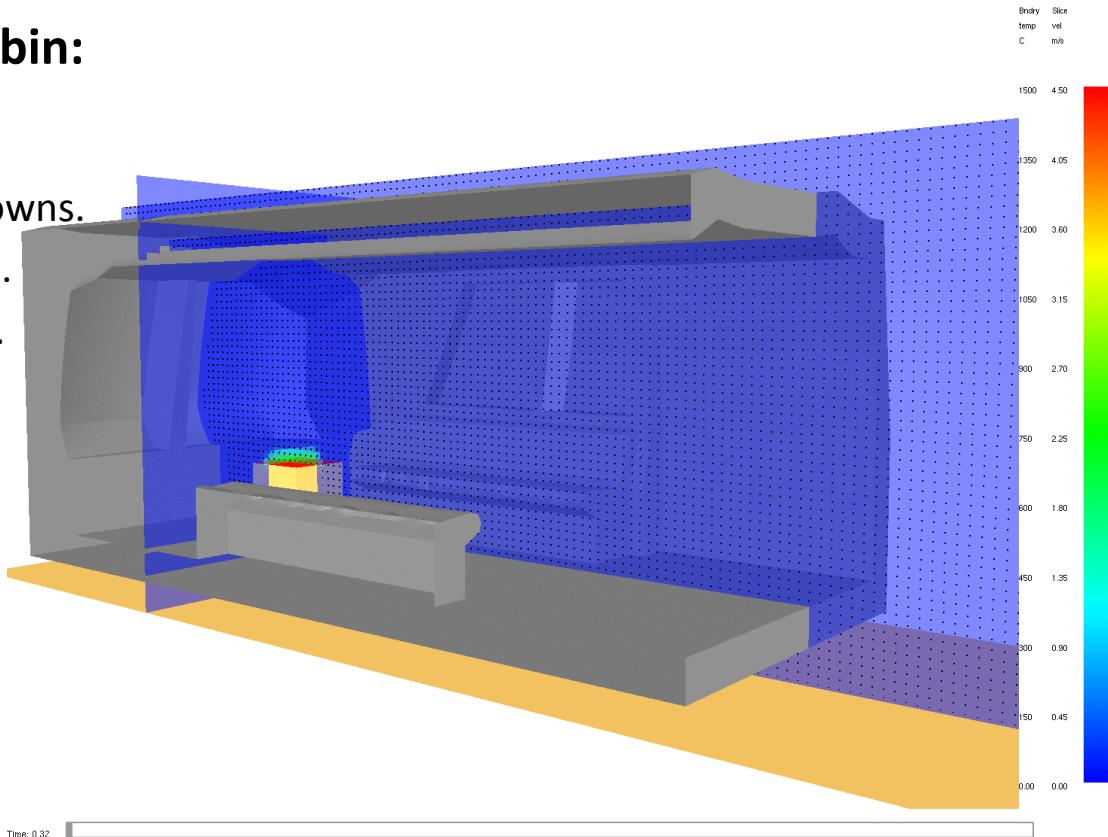
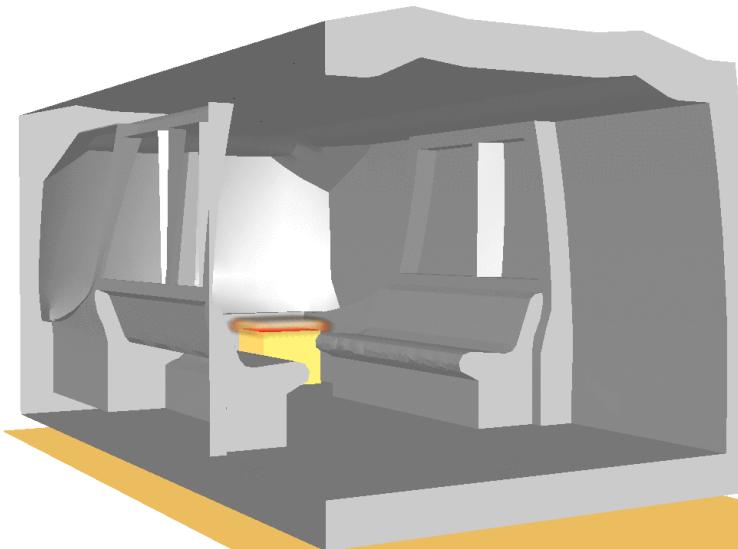
```
&HEAD CHID='cart_fire_800KW', TITLE='CC-IBM: Test propane fire on realistic train cart geometry.' /  
  
&MESH IJK=144,78,58, XB=-2.75,7.25,-2.25,2.25,-0.5,2.85 /  
  
&TIME T_END=50.0 /  
&MISC DNS=.FALSE.,  
NOISE=.FALSE.,  
STRATIFICATION=.FALSE.,  
CONSTANT_SPECIFIC_HEAT_RATIO=.FALSE.,  
BAROCLINIC=.FALSE.,  
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.

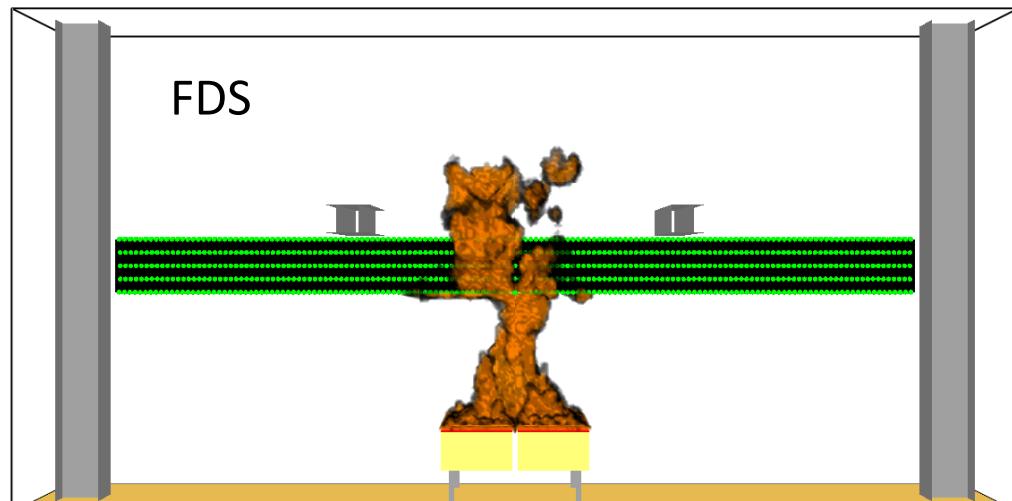
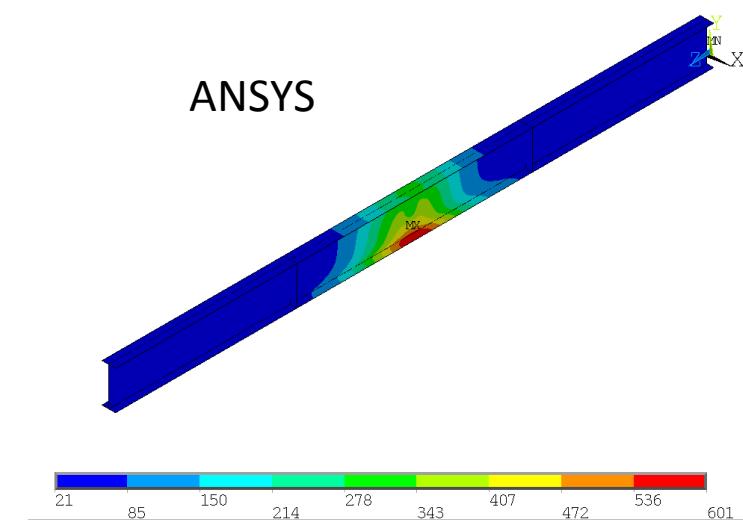


Smoke + HRRPUV contours.

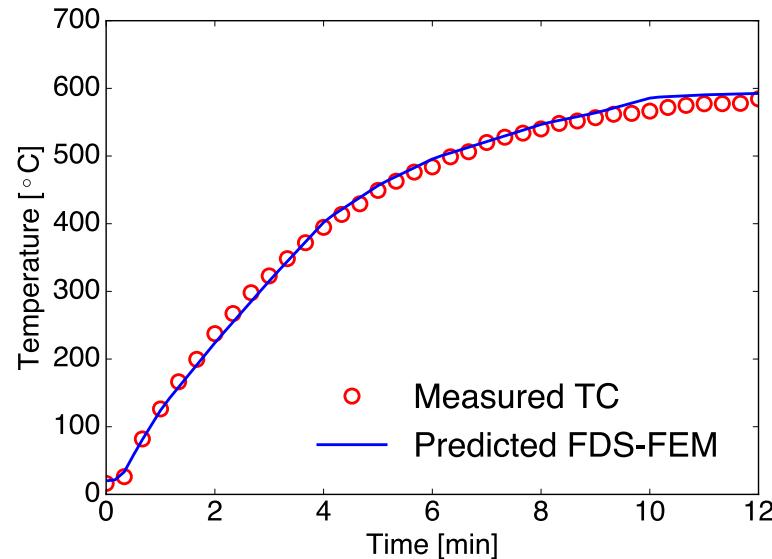
Future Work

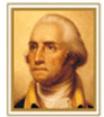


- Verification and Validation.
- Enhance radiation solver to solve RTE on cut-cells, add radiative boundary conditions on boundary cut-faces.
- Extend the treatment of particles from Cartesian cells unstructured cut-cells.
- Develop the data transfer for two way coupling with thermo-mechanical FEM solvers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



NFRL commissioning test, courtesy Chao Zhang.





Thank you