

Multi-material polygon based finite volume method for diffusion

MULTIMAT 2013, San Francisco, CA, 2nd–6th
September 2013

Alan Dawes (alan.dawes@awe.co.uk)



Outline

- Background
- Governing Equations
- Solution Strategy
 - Alternative Approach
 - Sub-cell Models
- Results
 - 1D: Linear Diffusion
 - 1D: Non-Linear Diffusion
 - 2D: Cylindrical Linear Diffusion
 - 2D: Cylindrical Non-Linear Diffusion
- Conclusions



Background

- ❑ For high speed flows simulations with large material distortions either the pure Eulerian or Arbitrary Lagrangian Eulerian (ALE) numerical methods can be used.
- ❑ For Inertial Confinement Fusion (ICF) simulations the governing equations are supplemented with source terms representing the diffusion of energy across material boundaries.
- ❑ The equations are solved numerically using operator splitting, with the diffusion terms treated separately from the hydrodynamics stage.
- ❑ Numerical methods based on Support Operators can be used to solve the diffusion equation but assume that the grid is aligned with the material boundaries.
- ❑ For ALE or Eulerian meshing the grid will not be, in general, aligned with the material boundaries.
- ❑ Cells that overlap material boundaries will contain more than one material component; known as a mixed cell.
- ❑ For diffusion, the most general approach is to treat pure and mixed cells alike. However, need to construct a dual *polygonal* mesh around the different materials.



Governing Equations

- For multi-material flow we wish to solve Partial Differential Equations with diffusive energy source term:-

$$\frac{\partial U_m}{\partial t} + \nabla \cdot \underline{F}_m = -\nabla \cdot \underline{D}_m$$

- The system is solved numerical using operator splitting thus:-

$$U_m = \begin{pmatrix} \rho_m \\ \rho_k \underline{u}_m \\ \rho_m E_m \end{pmatrix} \quad \underline{F}_m = \begin{pmatrix} \rho_m \underline{u}_m \\ \rho_m \underline{u}_m \underline{u}_m + p_m \\ \rho_m \underline{u}_m E_m + p_m \underline{u}_m \end{pmatrix}$$

- First step is the “homogeneous” Hydro step

$$\frac{\partial U_m}{\partial t} + \nabla \cdot \underline{F}_m = 0$$

$$\underline{D}_m = \begin{pmatrix} 0 \\ 0 \\ -K_m \nabla T_m^q \end{pmatrix}$$

- Second step is the Energy Diffusion Step

$$\frac{\partial \rho_m \epsilon_m}{\partial t} = \nabla \cdot (K_m \nabla T_m^q)$$

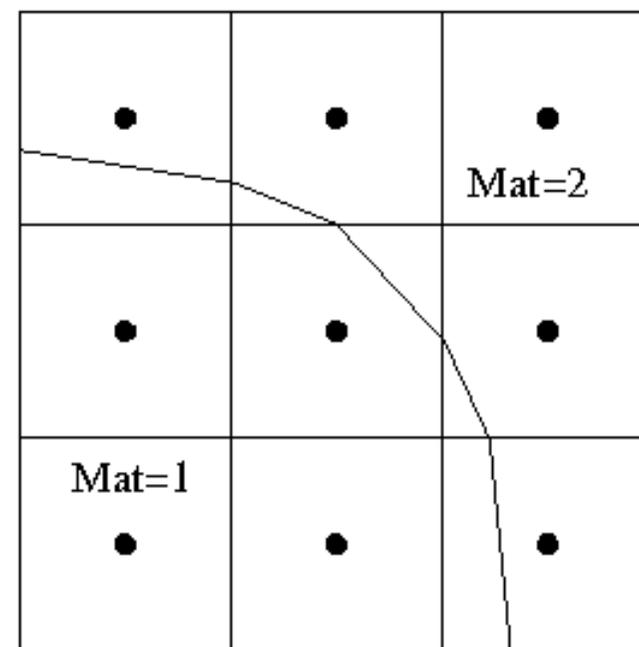
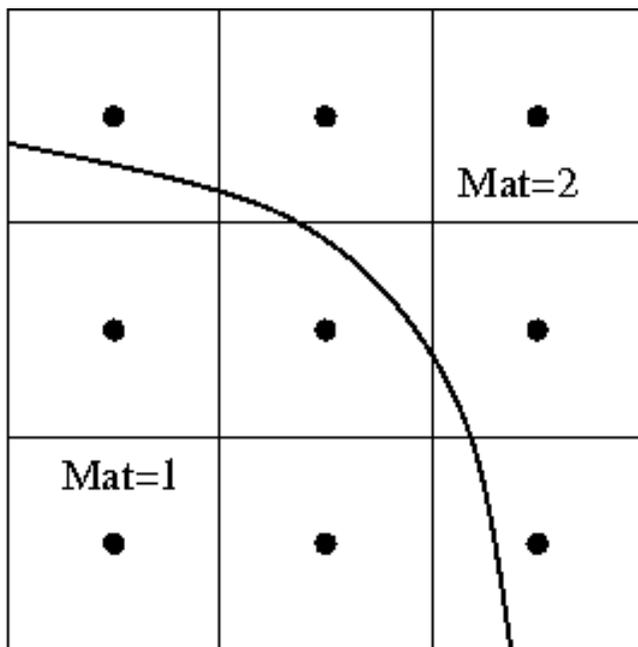
Hydro step based upon either Eulerian or ALE approach.

$$E_m = \epsilon_m + |\underline{u}|^2 / 2$$



Solution Strategy (1/4)

- ❑ Calculation setup with different materials.
- ❑ Material boundaries reconstructed using Volume of Fluid (VoF) Youngs' interface reconstruction.
- ❑ Material's have distinct properties
 - ❑ Pure and Mixed cell components have distinct properties.

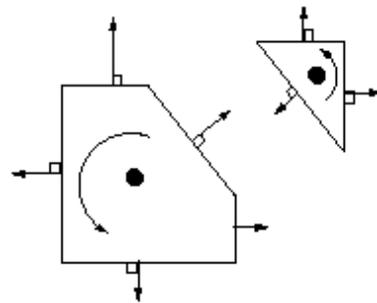
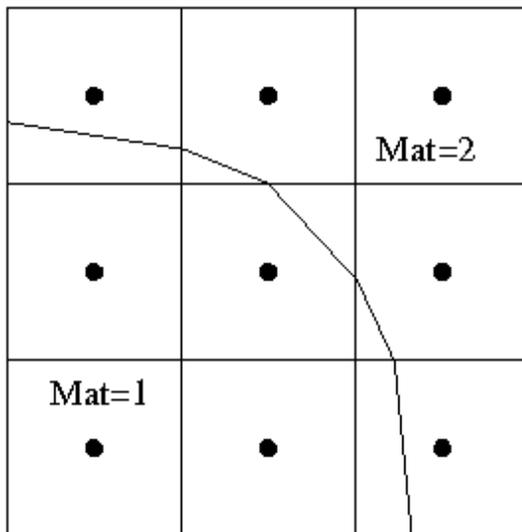


Solution Strategy (2/4)

□ Governing equation for m^{th} Component are integrated over time Δt and corresponding polygonal volume V_m

$$\frac{\partial \rho_m \varepsilon_m}{\partial t} = -\nabla \cdot \underline{F}_m \Rightarrow$$

$$\rho_m V_m (\varepsilon_m^{n+1} - \varepsilon_m^n) = -\Delta t \sum_{l=1}^{n\text{face}(m)} \underline{F}_{ml}^{n+\alpha} \cdot \underline{n}_{ml} \Delta S_{ml}$$



$$\underline{F}_{ml} = -K_{ml} \nabla \phi_{ml}$$

$$\phi = T^q$$

□ α indicates time centering used for temperature sub-cycling

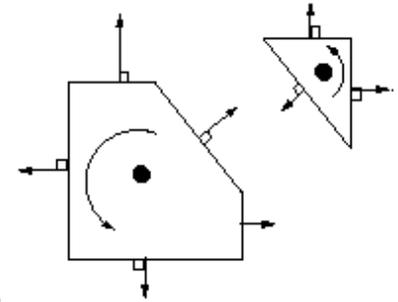
□ $\alpha=0$ (semi-implicit)

□ $\alpha=1/2$ (Picard)

□ $\alpha=1$ (full-implicit)

Solution Strategy (3/4)

$$\rho_m V_m (\epsilon_m^{n+1} - \epsilon_m^n) = -\Delta t \sum_{l=1}^{nface(m)} \underline{F}_{ml}^{n+\alpha} \cdot \underline{n}_{ml} \Delta S_{ml}$$



- ❑ Compute dual mesh that contains pure and mixed cells
 - ❑ Polygons
 - ❑ Number of faces
 - ❑ Connectivity to its neighbours
 - ❑ Inter-cell and Intra-cell values
 - ❑ Material Centroids
 - ❑ Inter-cell and Intra-cell lengths
- ❑ Creates connectivity array that is unstructured



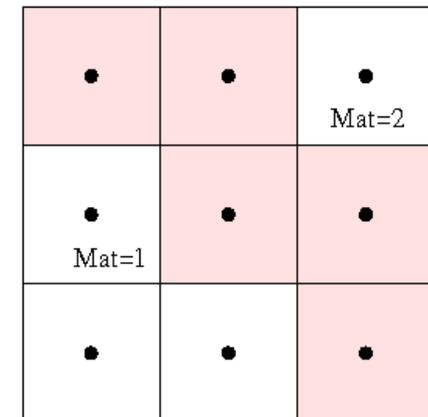
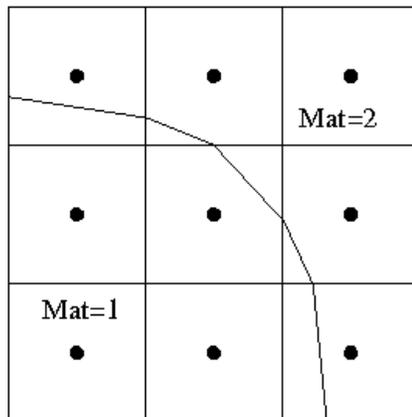
Solution Strategy (4/4)

- ❑ Solve as backward Euler system of implicit equations
 - ❑ Number of unknowns $N = n_{\text{pure}} + n_{\text{mixed_components}}$
- ❑ Linear system of equations $A^m \underline{u}^{m+1} = \underline{R}^m$
- ❑ A^m is a sparse $N \times N$ matrix, \underline{u}^{m+1} is the column vector of unknown temperatures and \underline{R}^m is the column vector for the right hand side, m is the iteration count
 - ❑ Temperature iterated until convergence
- ❑ Use HYPRE IJ (CSR format) due to unstructured nature of dual mesh
 - ❑ LLNL Library
 - ❑ Solver: Conjugate Gradient (CG)
 - ❑ Preconditioner: BoomerAMG (AMG)



Alternative Approach

- ❑ Homogenise “average” mixed cells to produce “pseudo” pure cells
 - ❑ Geometric simple than multi-material scheme
 - ❑ No need to compute dual mesh
 - ❑ Neighbours remain fixed but data changes
 - ❑ Matrix row and columns have fixed position but entries change
- ❑ Need for sub-cell improvements in mixed cells after main solve
 - ❑ “Solving the diffusion equation on a non-aligned mesh”, Computers and Fluids, May 2013





Sub-cell: Homogenized Model (HS)

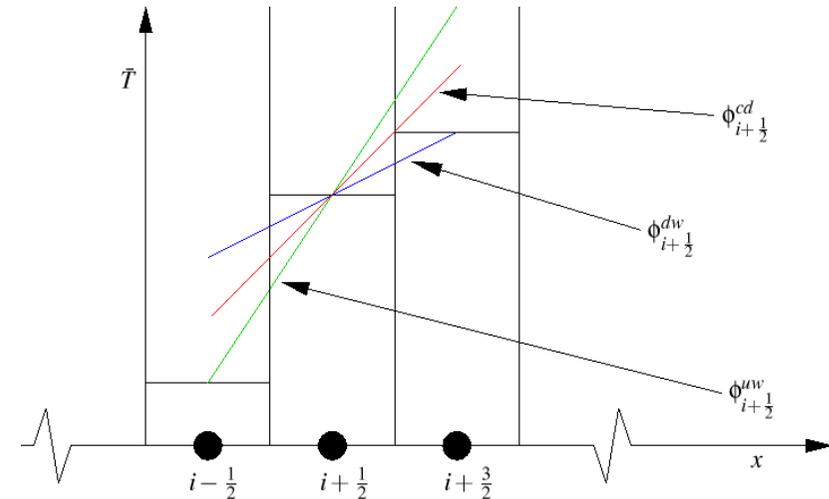
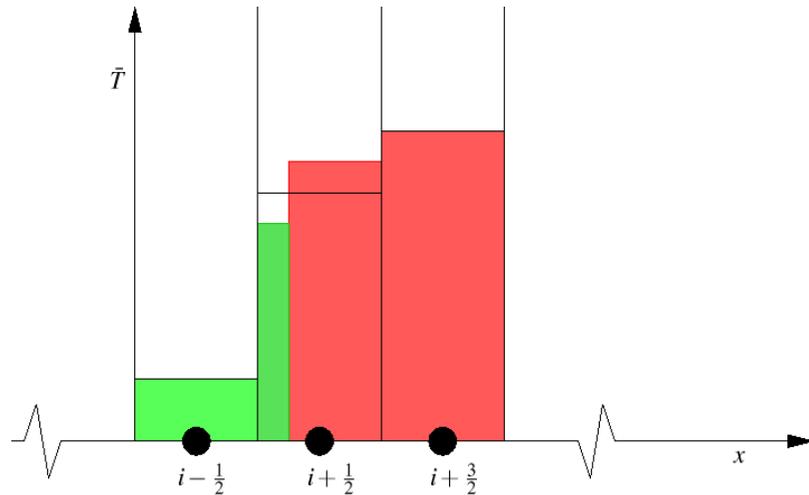
- Averaged temperature \overline{T}_c^{n+1} can be given to all mixed components
 - Instantaneous temperature equilibrium
- For consistency with the underlying energy equation the energy update follows the form,

$$\mathcal{E}_m^{n+1} = \mathcal{E}_m^n + C_{vm}^{n+1} \left(\overline{T}_c^{n+1} - T_m^n \right)$$

- Component values not \overline{T}_c^{n+1} but will eventually converge (few steps) to a single value.



Sub-cell: Gradient Based Model (GBM)



- Component temperatures are perturbed to maintain local energy conservation

$$\sum \rho_m f_m \varepsilon_m^{-n+1} = \sum \rho_m f_m \varepsilon_m^{n+1}$$

- For N components there is one equation for N unknowns. For two components a gradient based model can be adopted. For this we make the assumption that the internal mixed cell profile has the form (component 2 is related to 1):

$$T_2^{n+1} = T_1^{n+1} + \Delta T_\alpha \quad \Delta T_2^{n+1} - \Delta T_1^{n+1} = \Delta T_\alpha$$

- ΔT_α is the temperature change across the mixed cell based upon using the surrounding cells that bracket it.



Sub-cell: Flux Based Models (1/2)

- ❑ Gradient Based Model does not account for exchange of energy into mixed cell and within it.
- ❑ Energy update has to be consistent with underlying homogenized scheme
- ❑ Neumann BCs – prescribed fluxes (FBM)
 - ❑ Inter-cell Fluxes same as those from homogeised scheme
 - ❑ Energy conservative but method can be unrobust ☹
- ❑ Dirichlet BCs – prescribed temperatures
 - ❑ Mixed cell assumed to be bathed in local temperature bath
 - ❑ Non-conservative energy as inter-cell fluxes different to homogenised values ☹



Sub-cell: Flux Based Models (2/2)

- Dirichlet BCs – prescribed temperatures
 - Mixed cell bathed in surrounding temperature bath
 - Compute updated component energy and scale
- Scaled Energy Model 1 (FBMSE1)

$$\tilde{\epsilon}_m^{n+1} = \epsilon_m^n + \gamma_{vm}^{n+\alpha} (T_m^{n+1} - T_m^n)$$

- Scaled Energy Model 2 (FBMSE2)

$$\tilde{\epsilon}_m^{n+1} = \gamma \epsilon_m^{n+1}$$



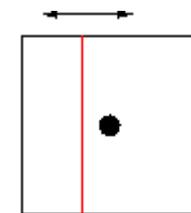
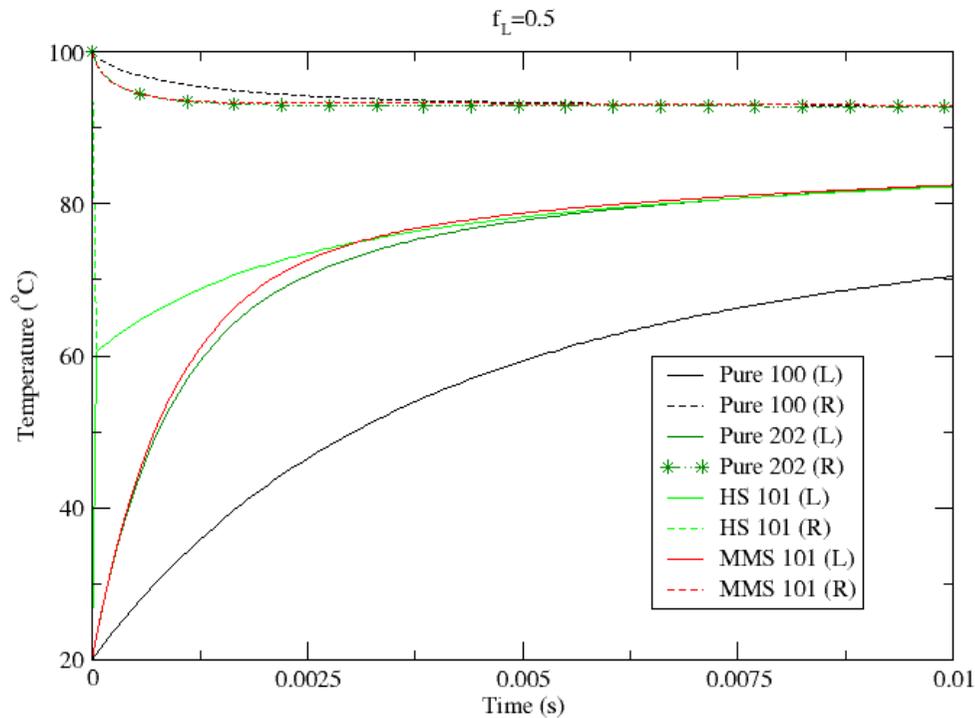
RESULTS

- ❑ HS: Homogenized Model
- ❑ GBM1: Gradient Based Model 1 ($\alpha \in [0,1]$)
- ❑ GBM2: Gradient Based Model 2
- ❑ FBM: Flux Based Model
- ❑ FBMSE1: Flux Based Model with Scaled Energy 1
- ❑ FBMSE2: Flux Based Model with Scaled Energy 2
- ❑ MMS: Multi-Material Scheme



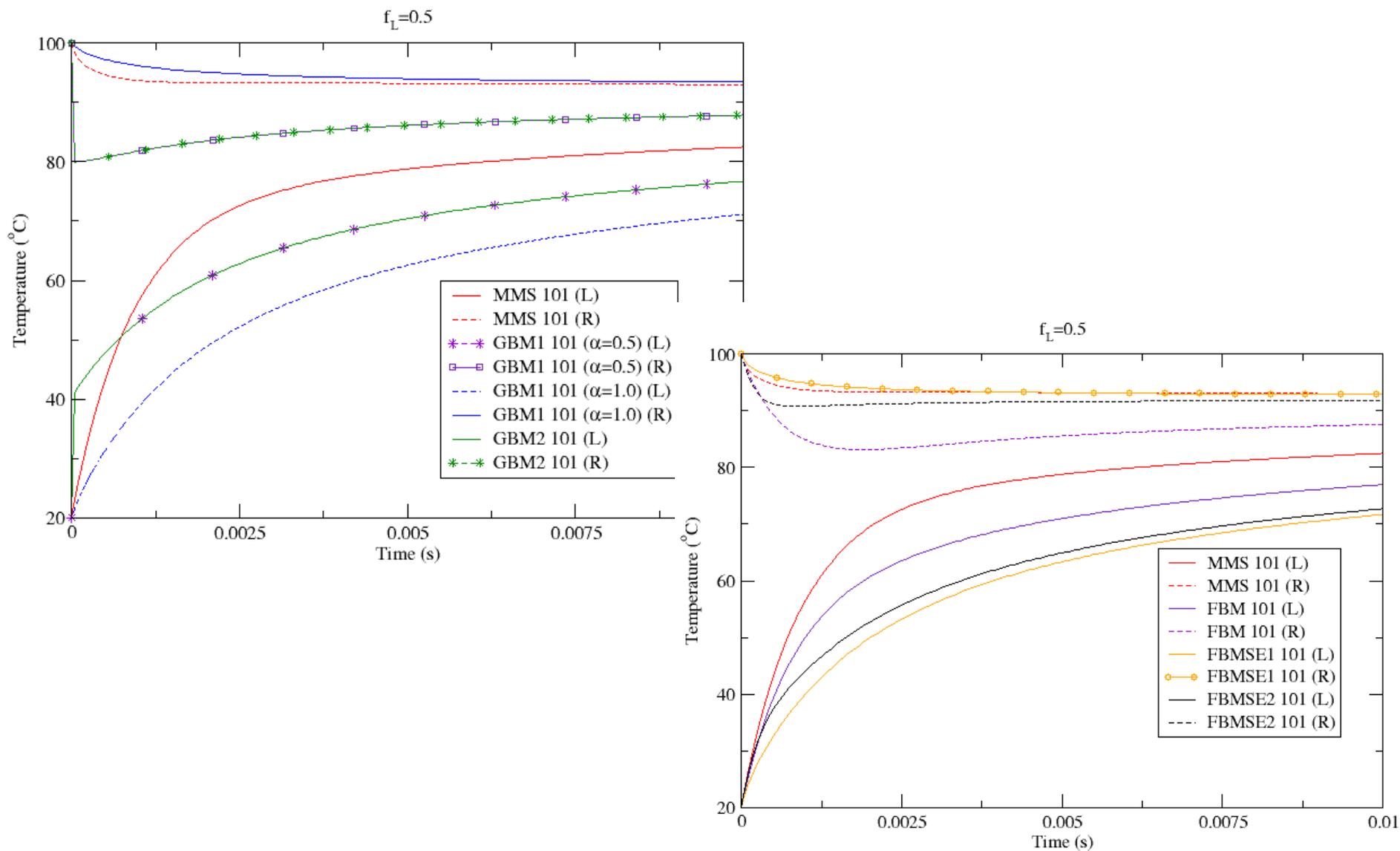
1D: Linear Diffusion

$$\begin{aligned}
 \frac{\partial T_L}{\partial t} &= \frac{\partial}{\partial x} \left(K_L \frac{\partial T_L}{\partial x} \right) & 0 \leq x < l/2 & & T_L = T_R & & x = l/2 & & T_L = 20^\circ \text{C} & & C_v = 1 \\
 \frac{\partial T_R}{\partial t} &= \frac{\partial}{\partial x} \left(K_R \frac{\partial T_R}{\partial x} \right) & l/2 < x \leq l & & K_L \frac{\partial T_L}{\partial x} = K_R \frac{\partial T_R}{\partial x} & & x = l/2 & & T_R = 100^\circ \text{C} & & q = 1 \\
 & & & & & & & & & & K_L = 0.01 & & K_R = 1
 \end{aligned}$$



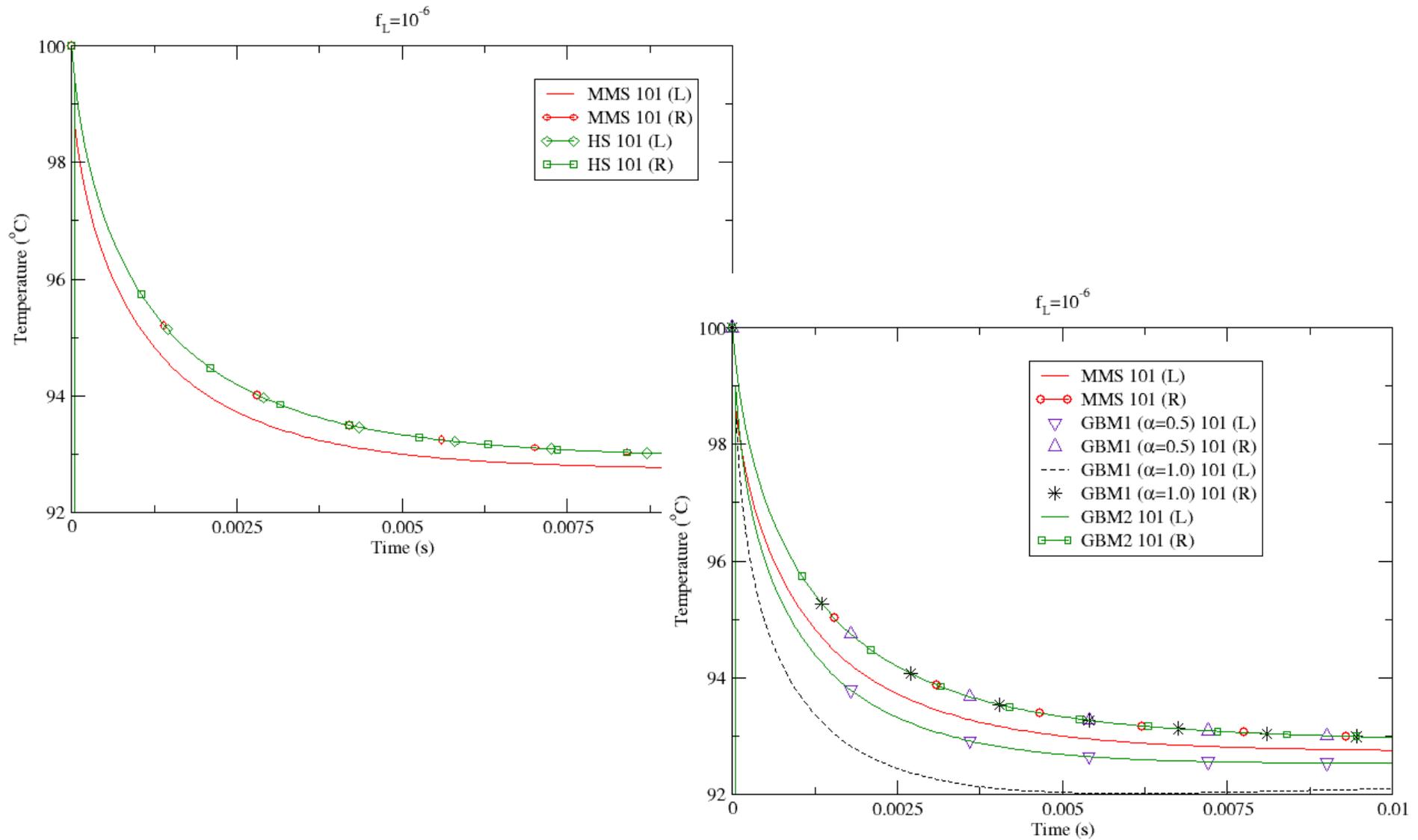


1D: Linear Diffusion



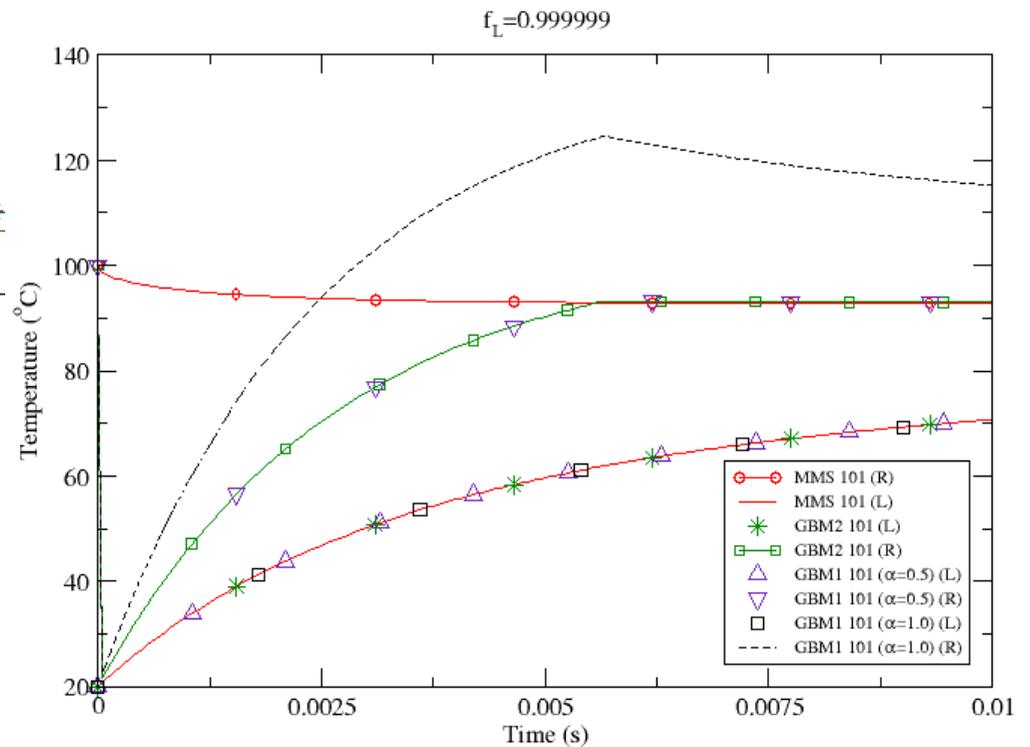
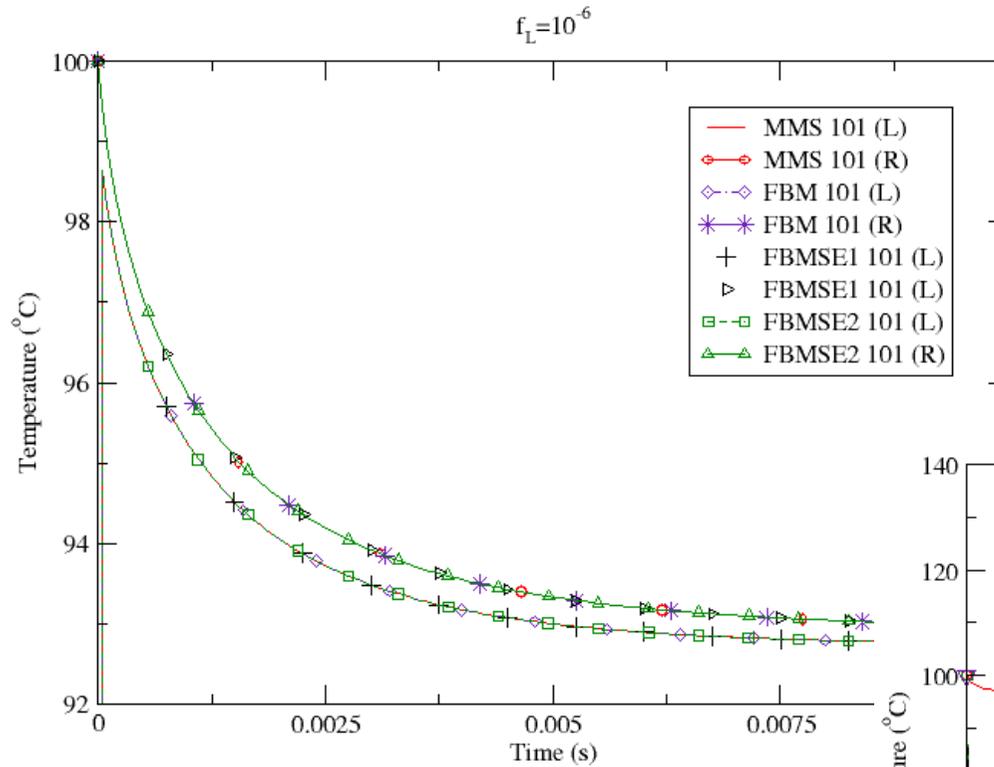


1D: Linear Diffusion



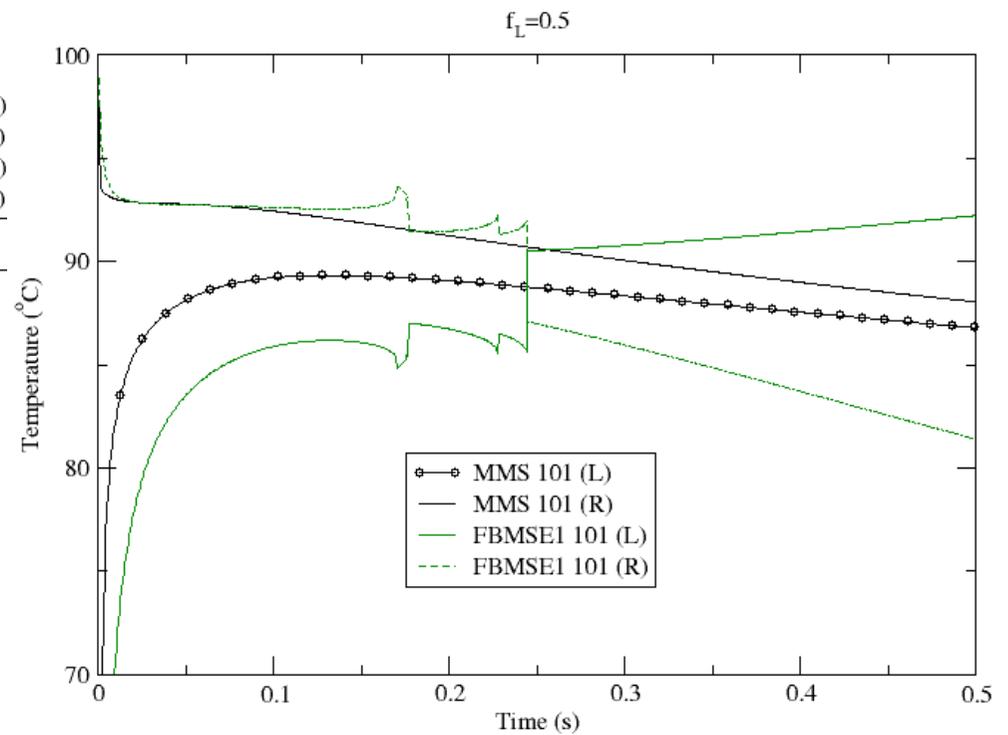
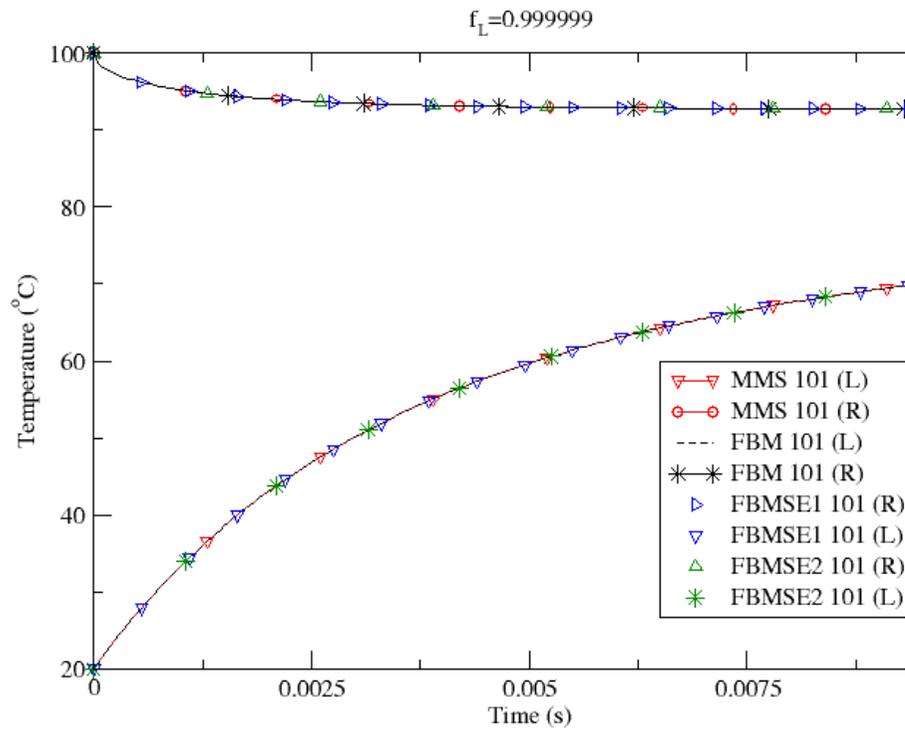


1D: Linear Diffusion



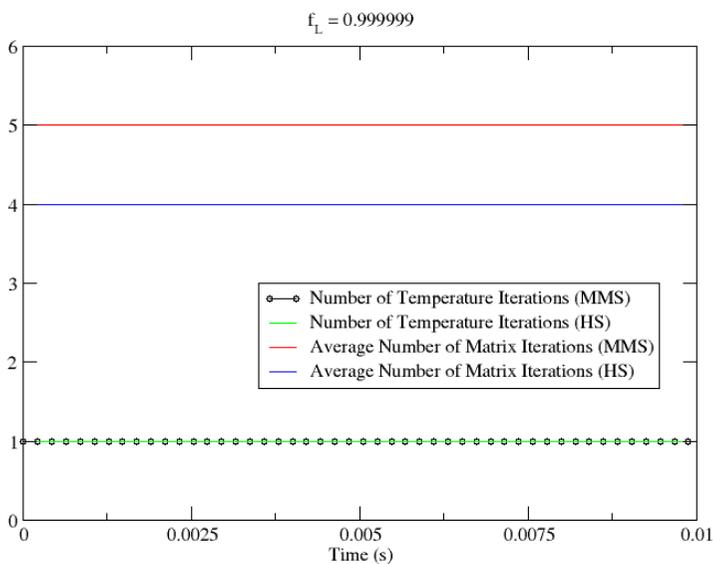
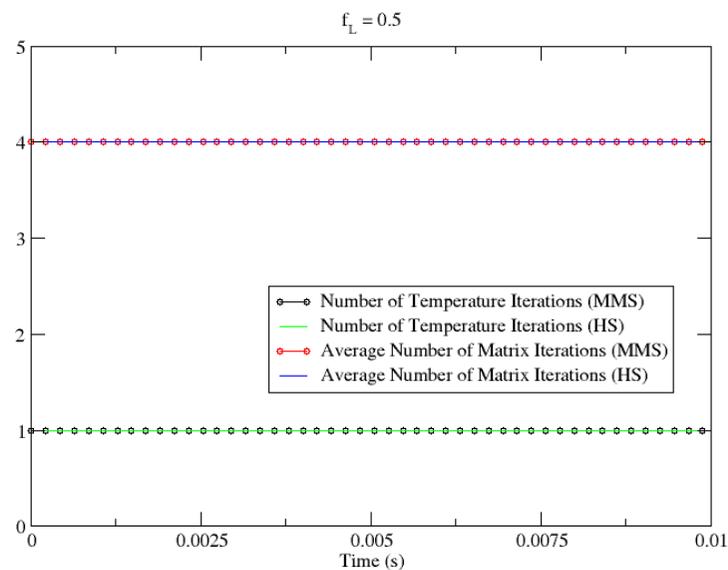
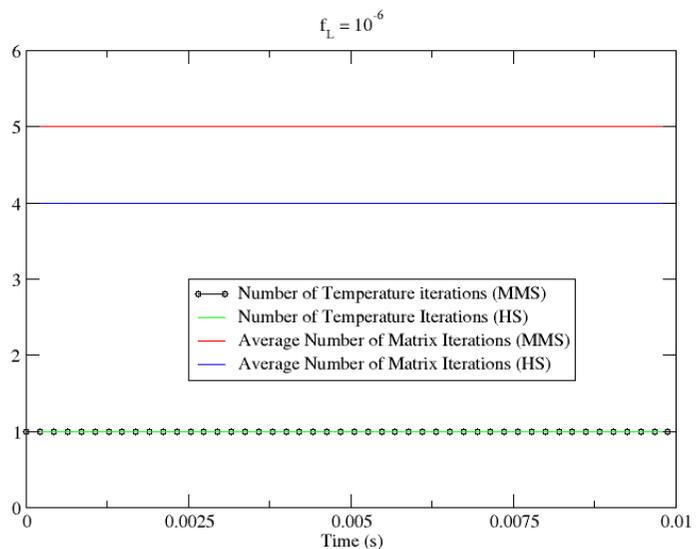


1D: Linear Diffusion





1D: Linear Diffusion



	MMS	HS	OTHERS
Compute Cost	0.88		
CDMPI	0.12		
Total Cost	1.0	0.75	~0.75



1D: Linear Diffusion

- ❑ GBM1, GBM2 and FBMSE1 performed poorly against MMS
- ❑ Models will not be considered any further



1D: Non-Linear Diffusion

$$\frac{\partial T_L}{\partial t} = \frac{\partial}{\partial x} \left(K_L \frac{\partial T_L^4}{\partial x} \right) \quad 0 \leq x < l/2$$

$$\frac{\partial T_R}{\partial t} = \frac{\partial}{\partial x} \left(K_R \frac{\partial T_R^4}{\partial x} \right) \quad l/2 < x \leq l$$

$$K_L \frac{\partial T_L^4}{\partial x} = K_R \frac{\partial T_R^4}{\partial x} \quad x = l/2$$

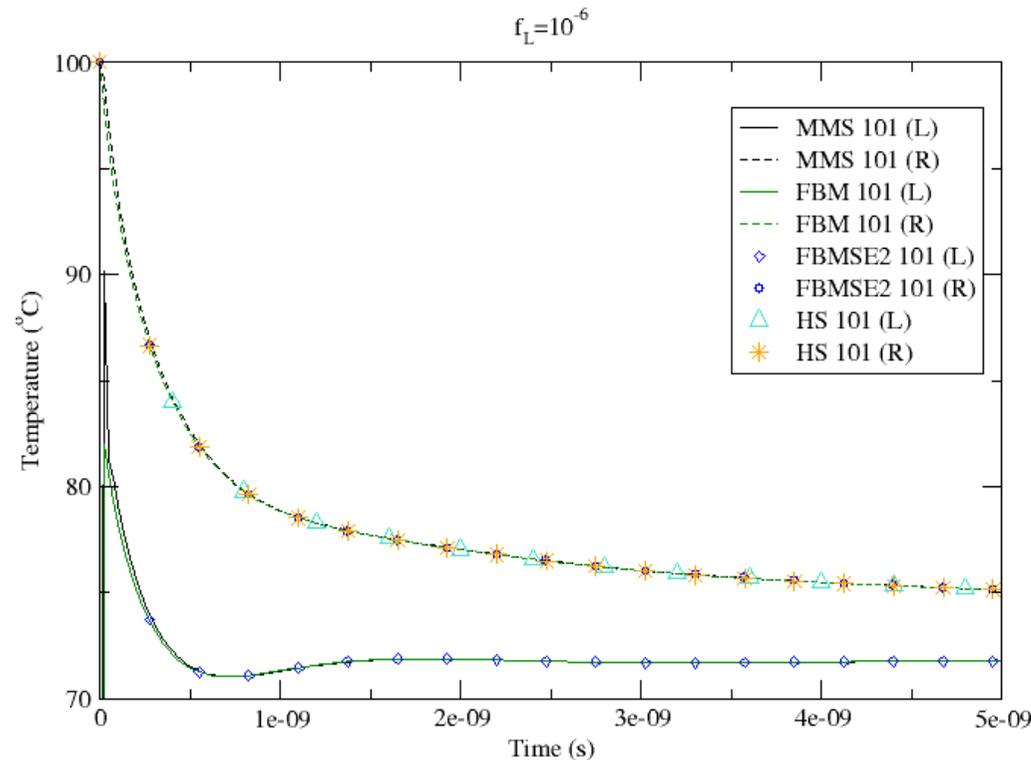
$$T_L = T_R \quad x = l/2$$

$$T_L = 20^\circ C$$

$$T_R = 100^\circ C$$

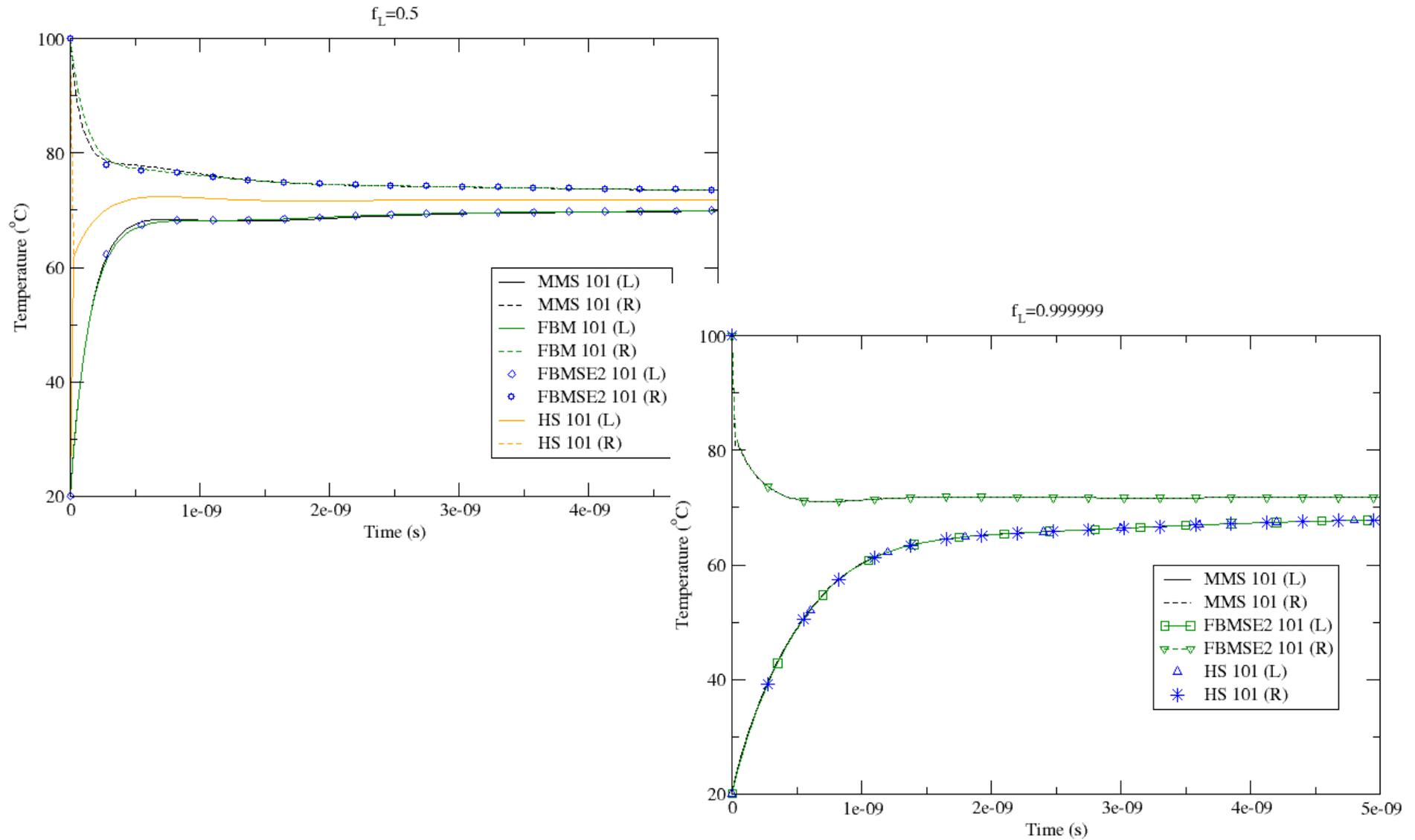
$$K_L = K_R = 0.1$$

$$C_v = 1 \quad q = 4$$





1D: Non-Linear Diffusion





1D: Non-Linear Diffusion

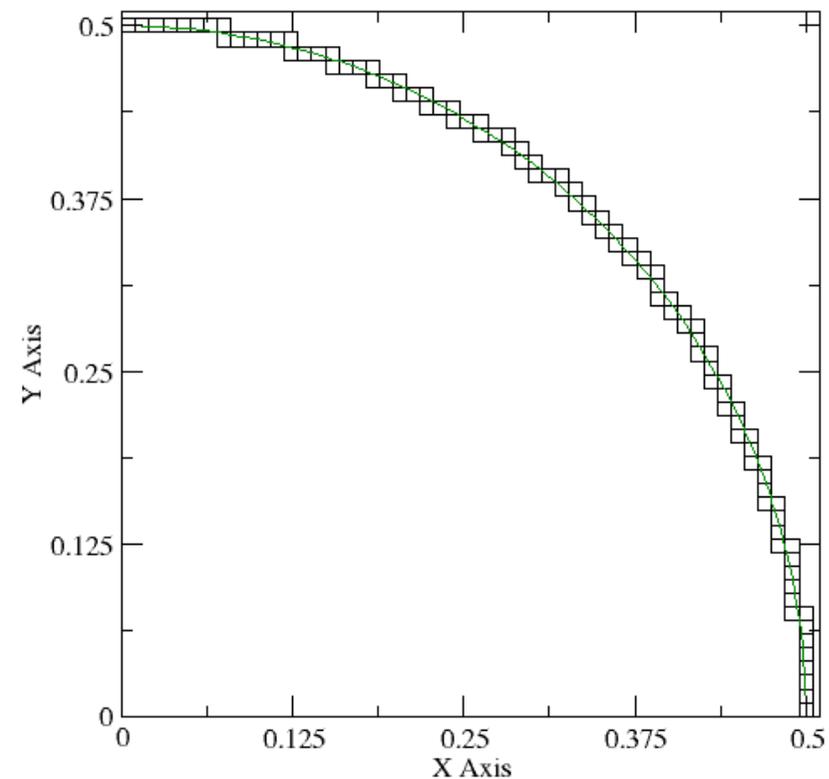
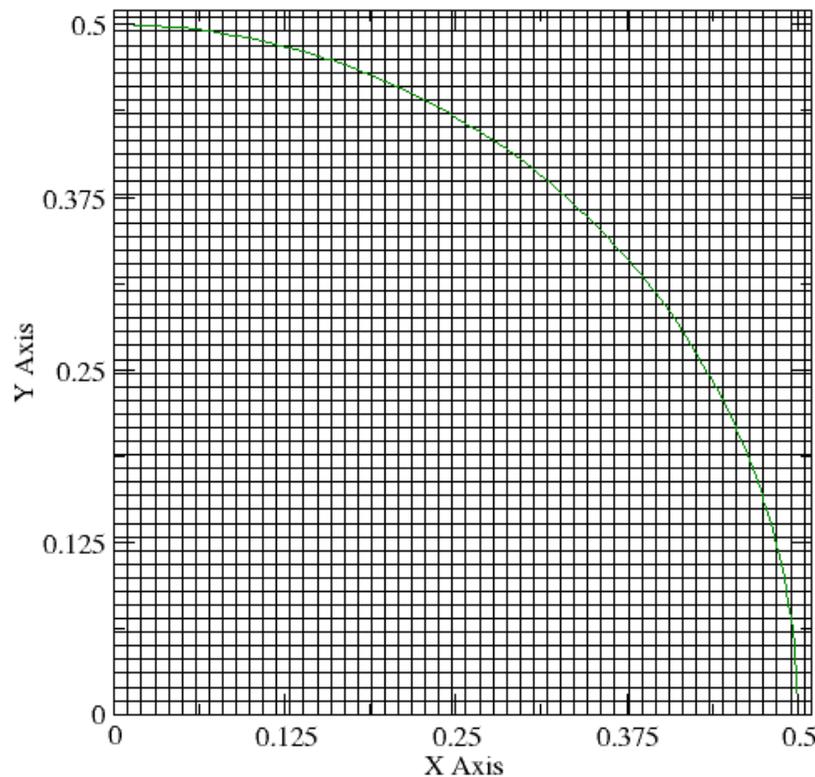
	MMS	HS	OTHERS
Compute Cost	0.87		
CDMPI	0.13		
Total Cost	1.0	0.70	~0.70

- ❑ FBM failed for $f_L = 0.999999$
- ❑ Model will not be considered any further



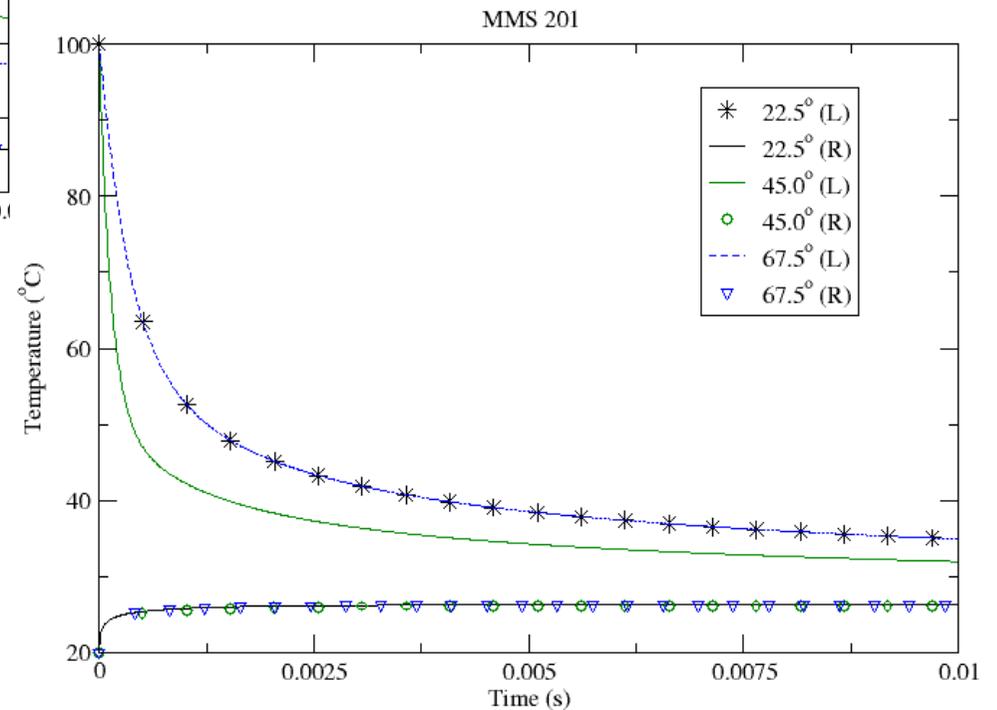
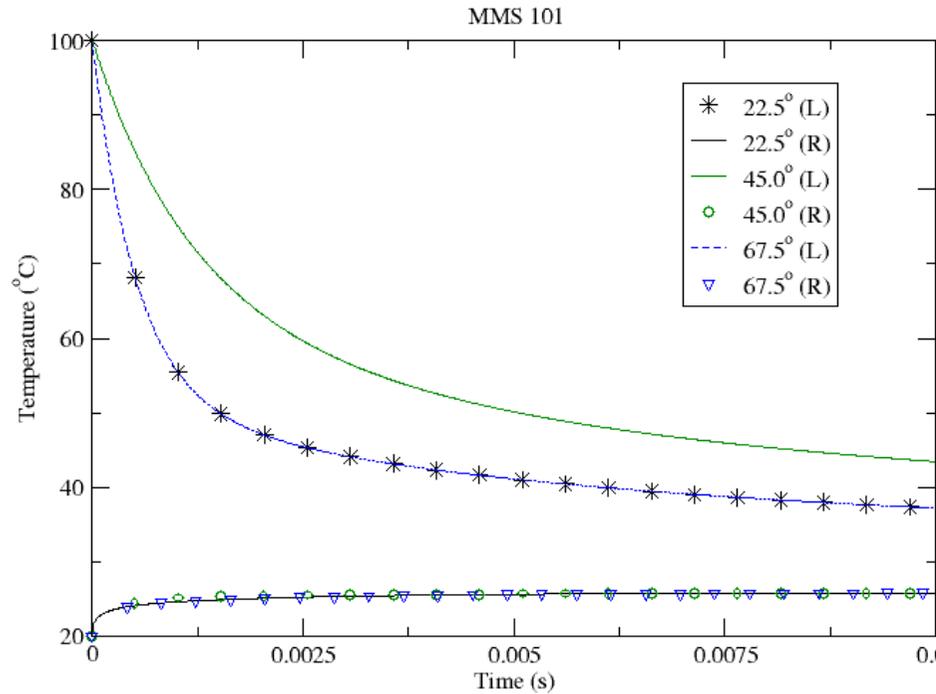
2D: Cylindrical Linear Diffusion

$$\begin{aligned} \frac{\partial T_L}{\partial t} &= \frac{\partial}{\partial x} \left(K_L \frac{\partial T_L}{\partial x} \right) & 0 \leq x < l/2 & \quad K_L \frac{\partial T_L}{\partial x} = K_R \frac{\partial T_R}{\partial x} & \quad x = l/2 & \quad T_L = 100^\circ C \quad K_L = 0.01 \\ \frac{\partial T_R}{\partial t} &= \frac{\partial}{\partial x} \left(K_R \frac{\partial T_R}{\partial x} \right) & l/2 < x \leq l & \quad T_L = T_R & \quad x = l/2 & \quad T_R = 20^\circ C \quad K_R = 1.0 \end{aligned}$$



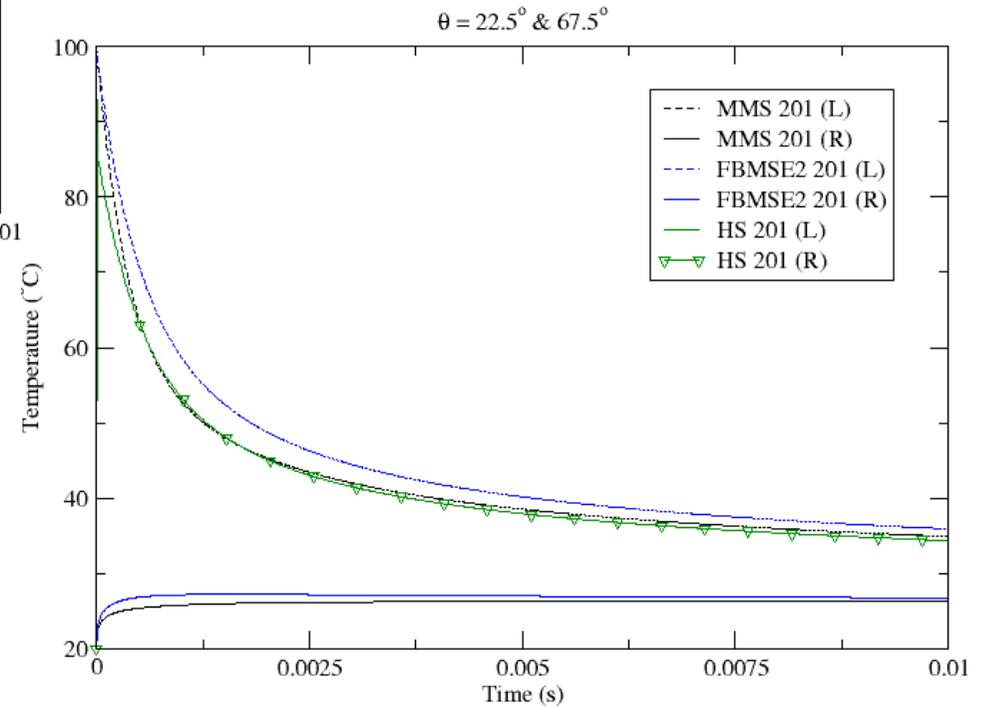
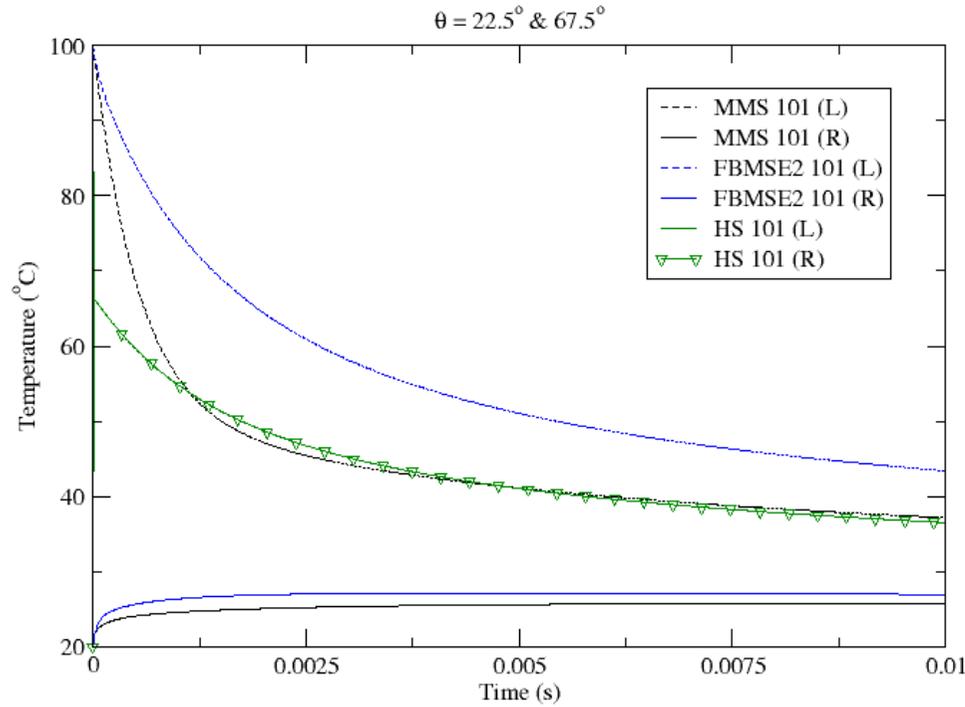


2D: Cylindrical Linear Diffusion



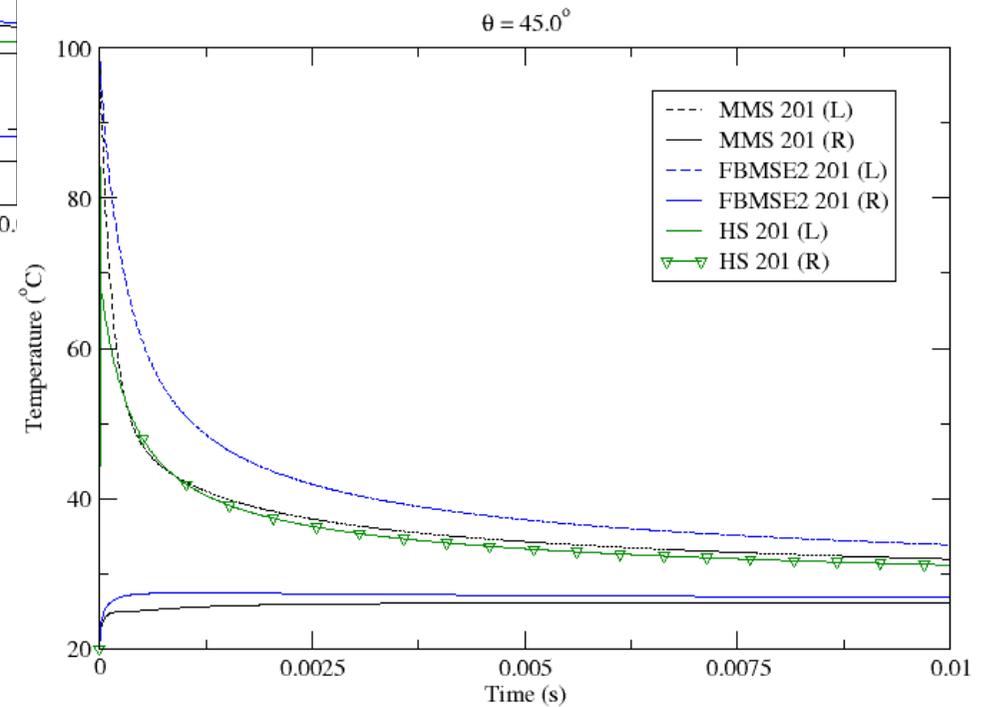
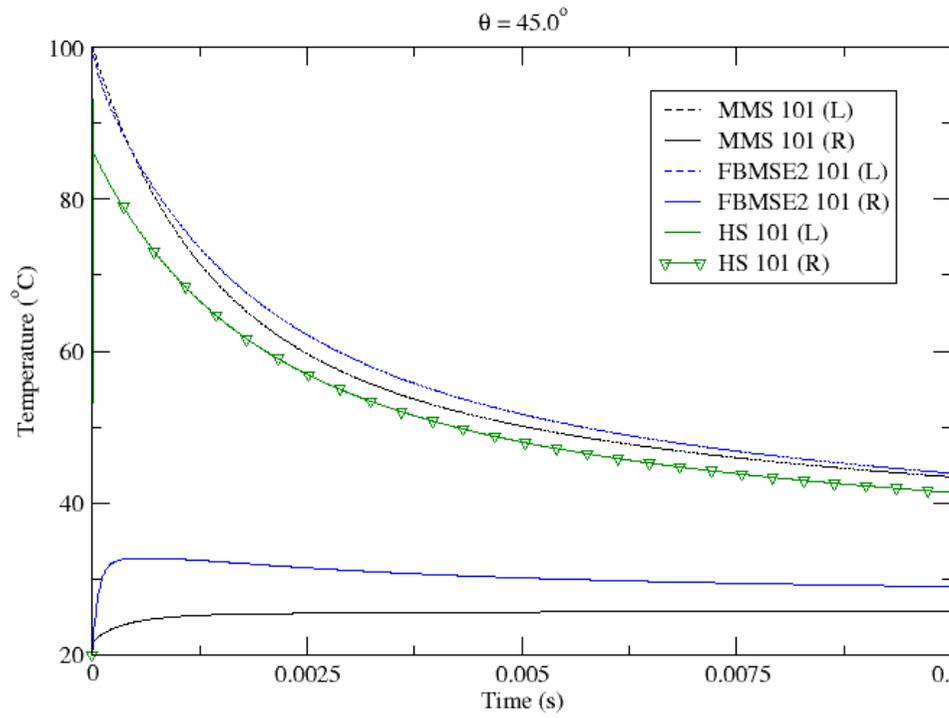


2D: Cylindrical Linear Diffusion





2D: Cylindrical Linear Diffusion





2D: Cylindrical Non-Linear Diffusion

$$\frac{\partial(10T_L^2)}{\partial t} = \frac{\partial}{\partial x} \left(K_L \frac{\partial T_L^4}{\partial x} \right) \quad 0 \leq x < l/2$$

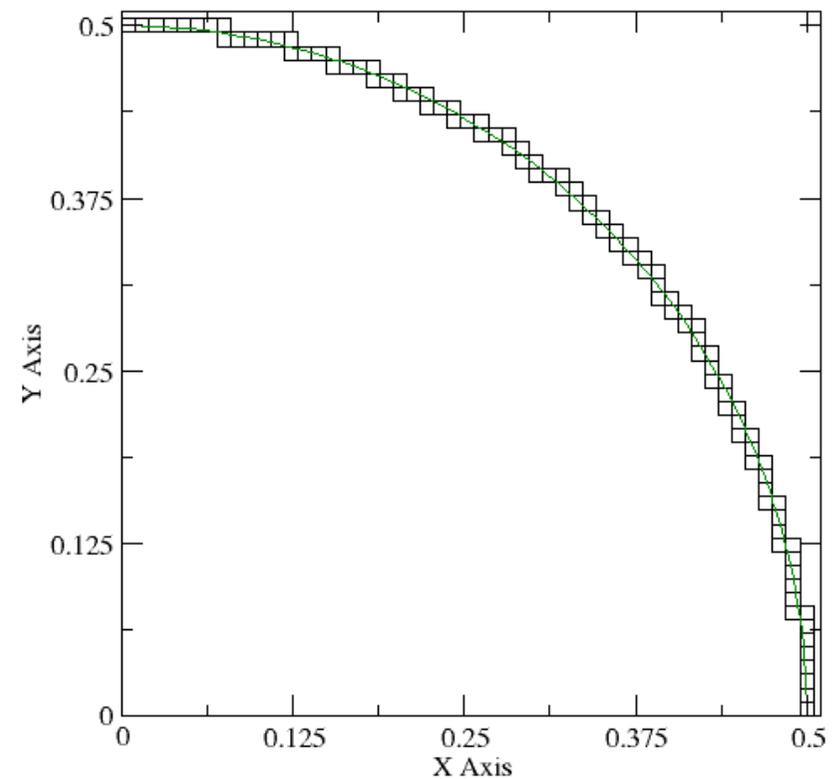
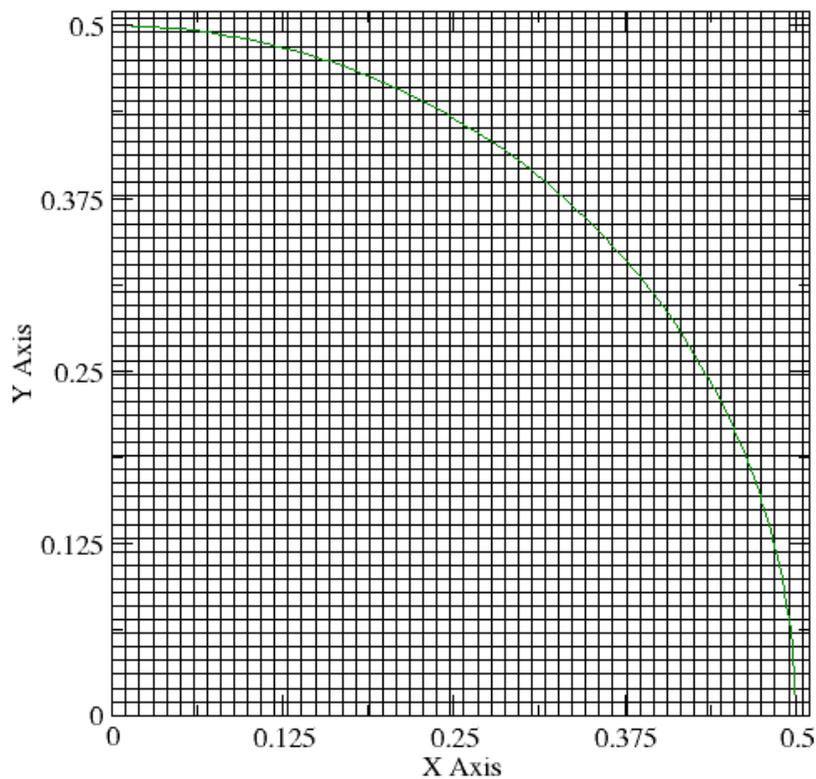
$$K_L \frac{\partial T_L^4}{\partial x} = K_R \frac{\partial T_R^4}{\partial x} \quad x = l/2 \quad T_R = 20^\circ C$$

$$T_L = T_R \quad x = l/2 \quad T_L = 100^\circ C$$

$$\frac{\partial T_R^2}{\partial t} = \frac{\partial}{\partial x} \left(K_R \frac{\partial T_R^4}{\partial x} \right) \quad l/2 < x \leq l$$

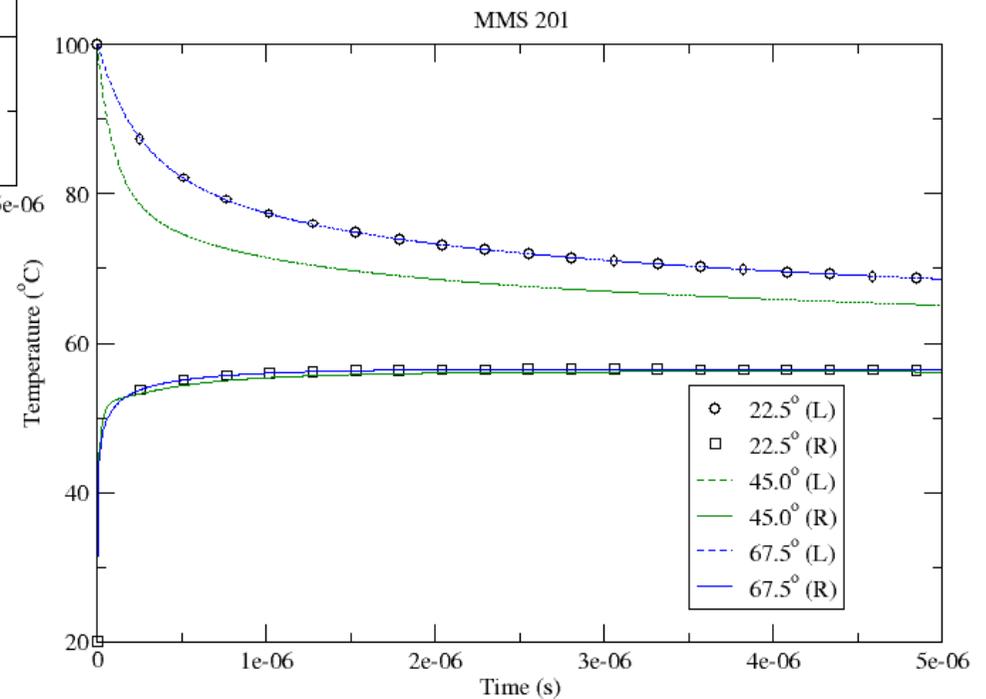
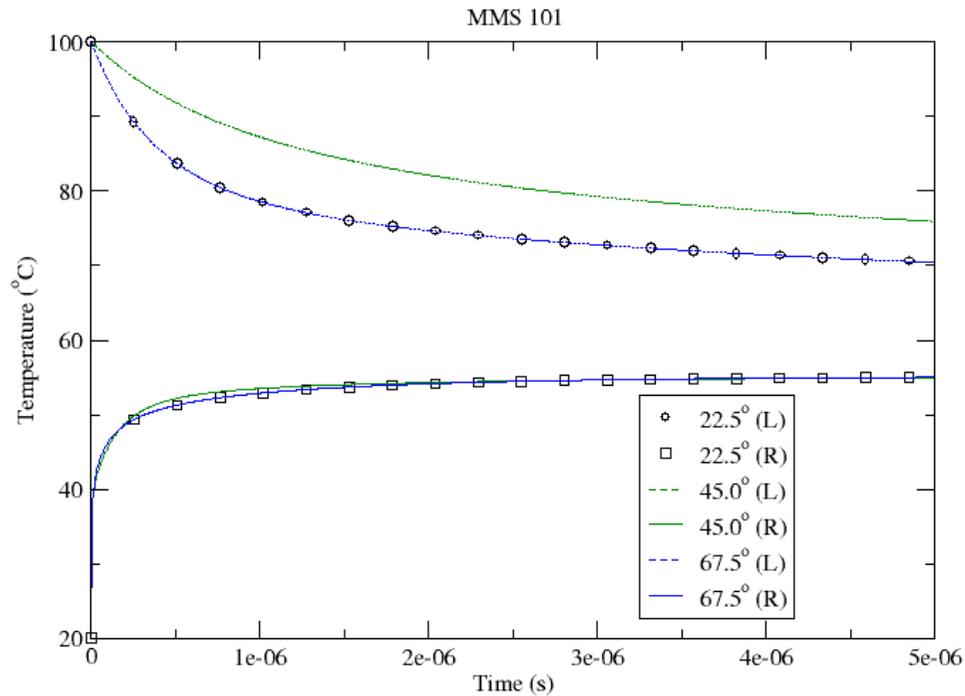
$$K_r = 0.01$$

$$q = 4 \quad K_R = 1.0$$



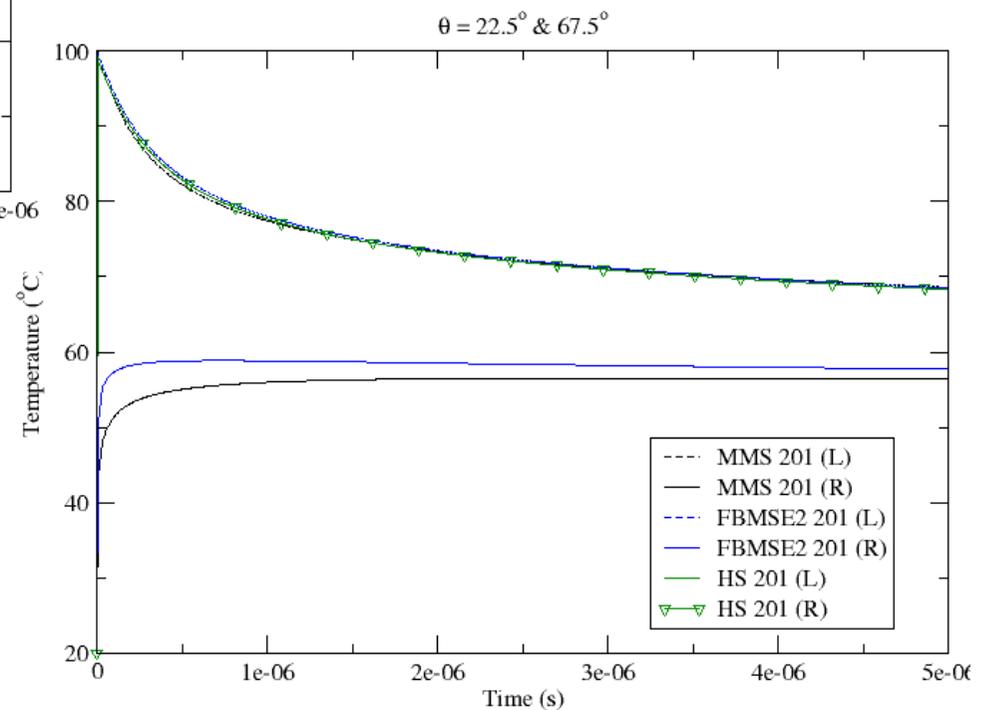
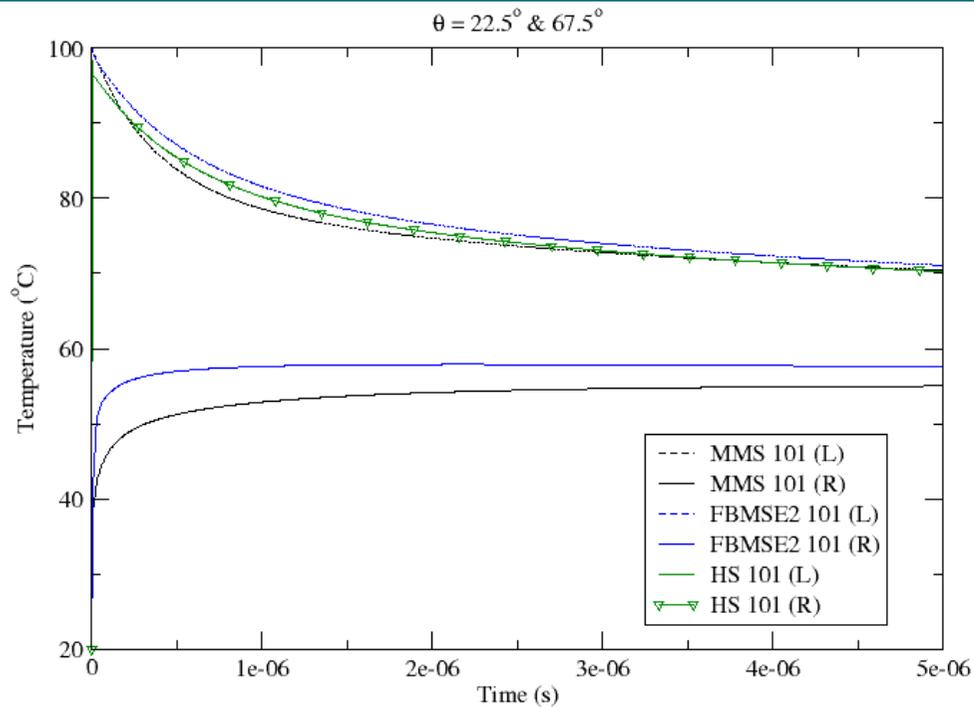


2D: Cylindrical Non-Linear Diffusion



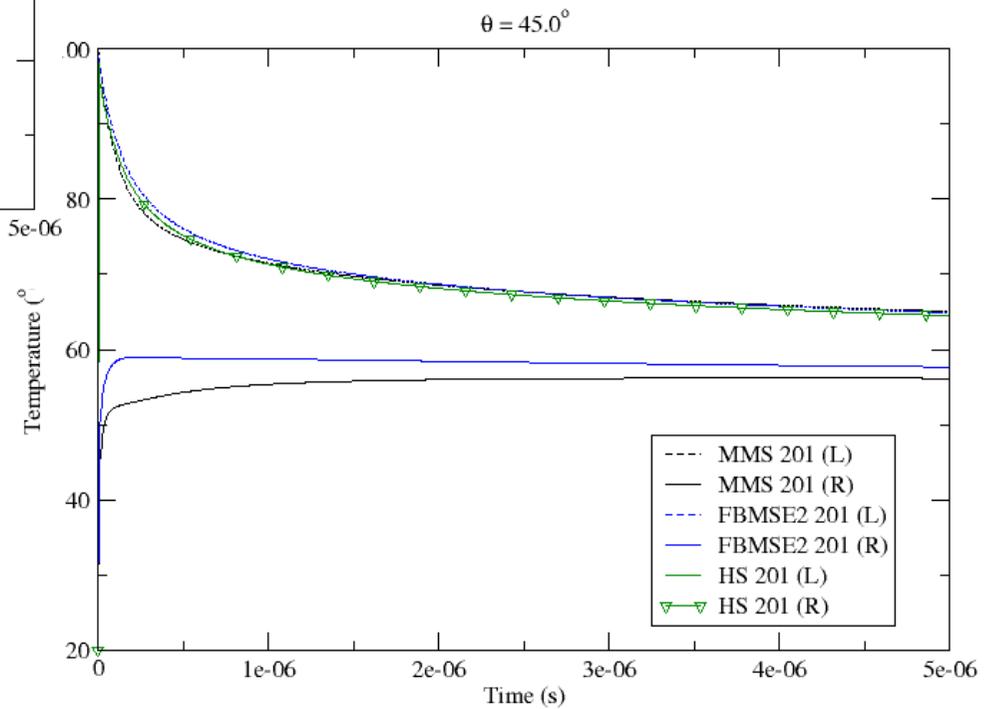
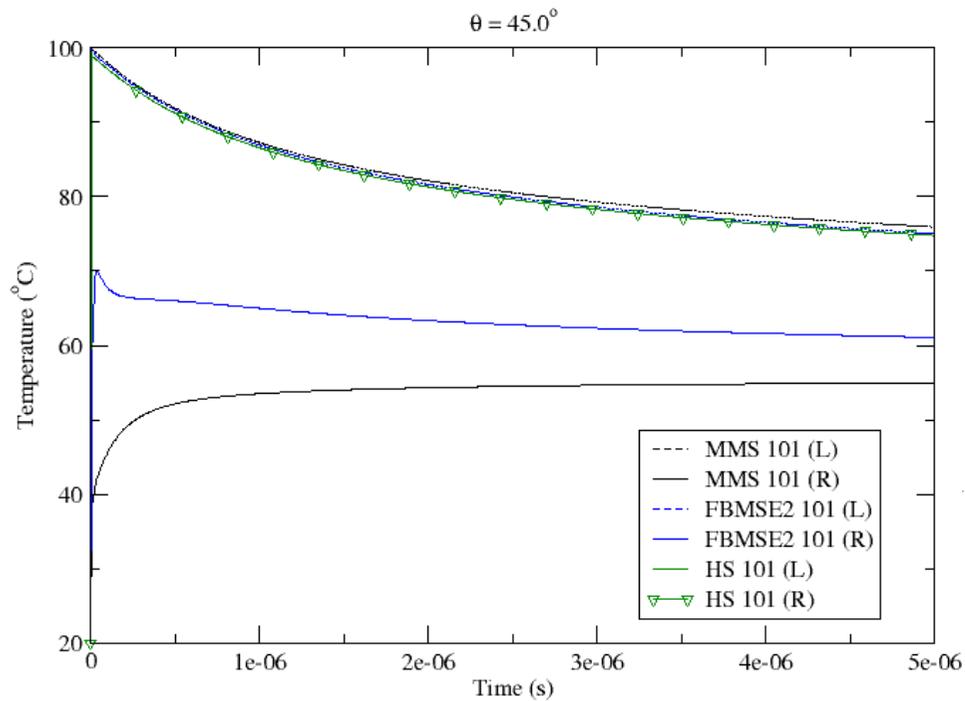


2D: Cylindrical Non-Linear Diffusion



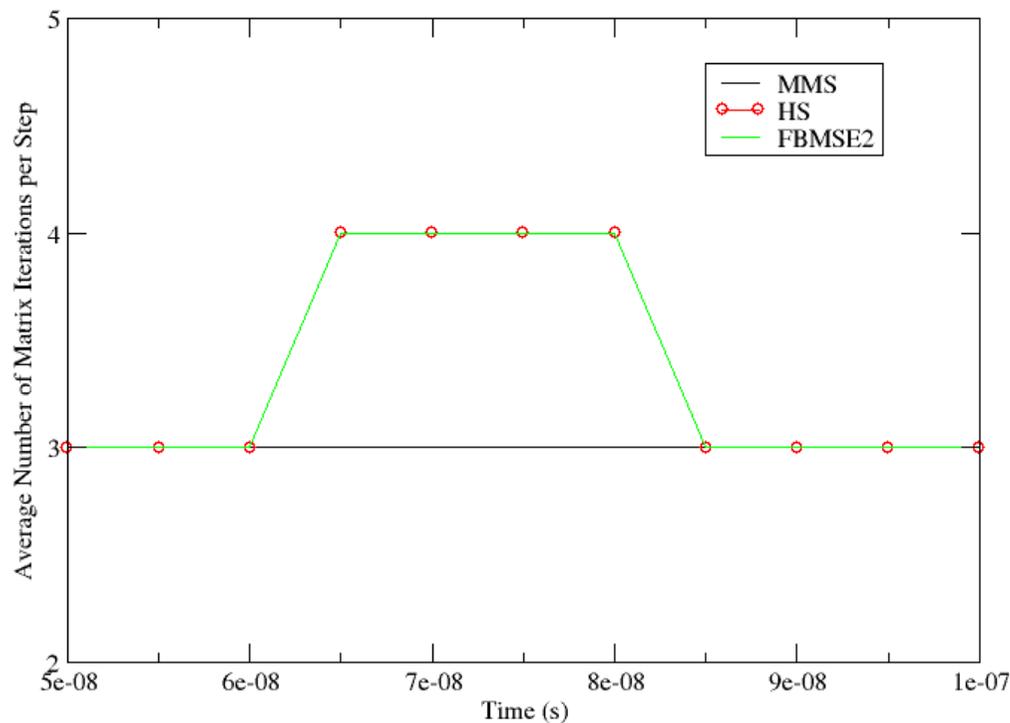


2D: Cylindrical Non-Linear Diffusion





2D: Cylindrical Non-Linear Diffusion



	MMS		HS		FBMSE2	
	101	201	101	201	101	201
Compute Cost	0.93	0.95	0.63	0.65	~0.97	~1.0
CDMPI	0.07	0.05	-	-	-	-
Total Cost	1.0	1.0	0.63	0.65	~0.97	~1.0



Conclusions

- ❑ A multi-material scheme for diffusion was presented
 - ❑ Necessary to compute on unstructured dual mesh (Polygons)
 - ❑ Additional geometric complexity, but best approach to capture inter-cell and intra-cell energy diffusion across material interfaces
- ❑ An alternative approach based on homogenization was presented
 - ❑ Several sub-cell models were described that aim to correct for the homogenization energy error
- ❑ Using simple test problems a process of elimination was used to identify the “best” sub-cell model relative to the multi-material scheme
- ❑ Homogenization error will always limit the sub-cell model accuracy
 - ❑ Multi-material scheme does not suffer from this