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DECOUPLED DISCRETIZATION OF PLASMA-MATERIAL INTERFACES IN MULTIPHYSICS PIC SIMULATIONS

An algorithm for non-conformal meshing and information transfer

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OUTLINE

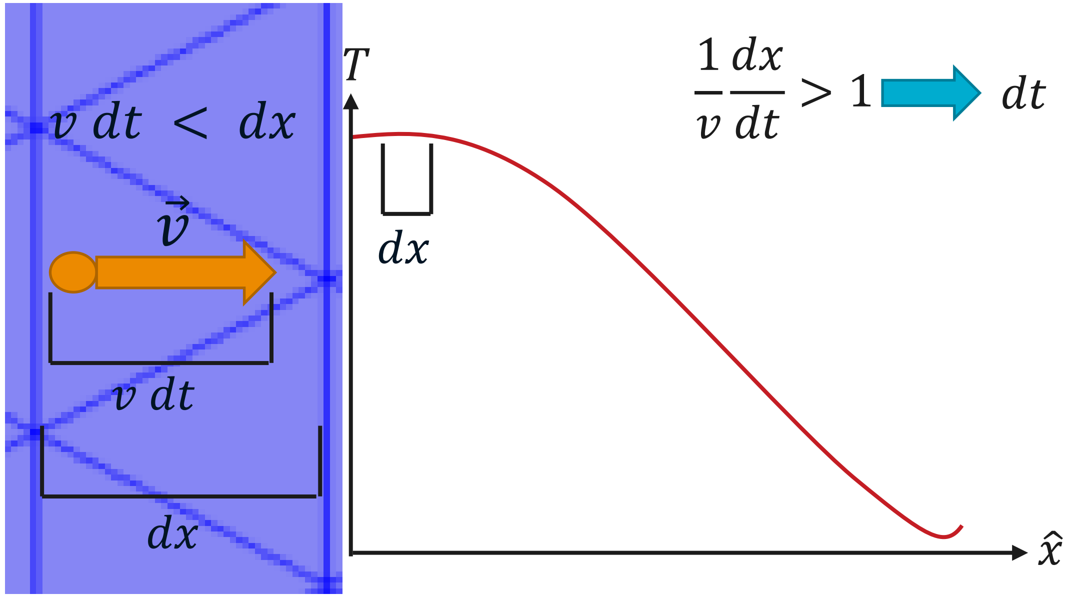
- Constraints on multiphysics Particle-In-Cell (PIC) simulations

- Spatial Discretization Decoupling Algorithm
  - Non-conformal mesh design
  - Pre-processing two-way mapping across non-conformal interfaces

- Multiphysics PIC simulations using Decoupling Algorithm
  - Thermal conduction by particle heat flux in quasi-1D, 2D, and 3D
  - Conformal meshes vs non-conformal meshes, convergence, and efficacy

- Conclusions

CONSTRAINTS ON MESHING IN PARTICLE-IN-CELL (PIC) SIMULATIONS LIMIT MULTIPHYSICS MODELLING.



- In high power vacuum arcs, the plasma and surrounding surfaces are strongly coupled (energy deposition, particle emission, surface modification). Particle to surface heat conduction demonstrates this (top).

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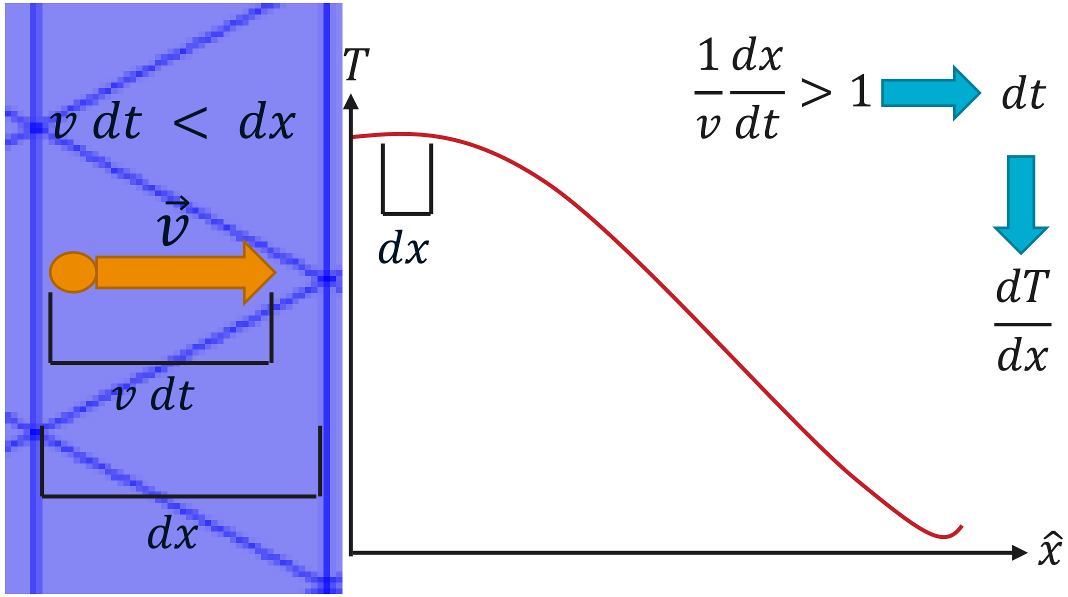

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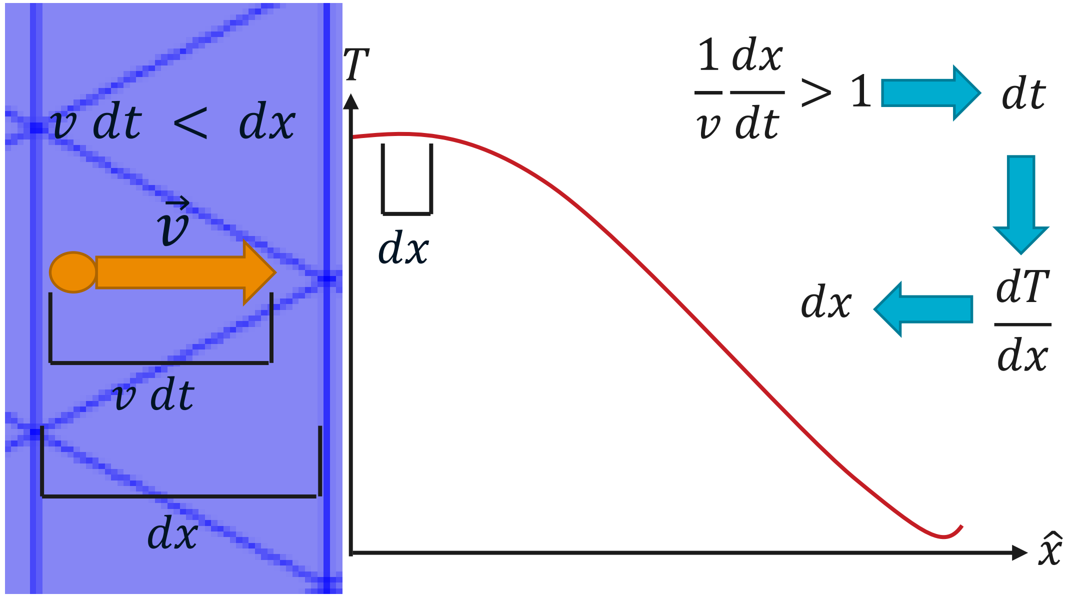

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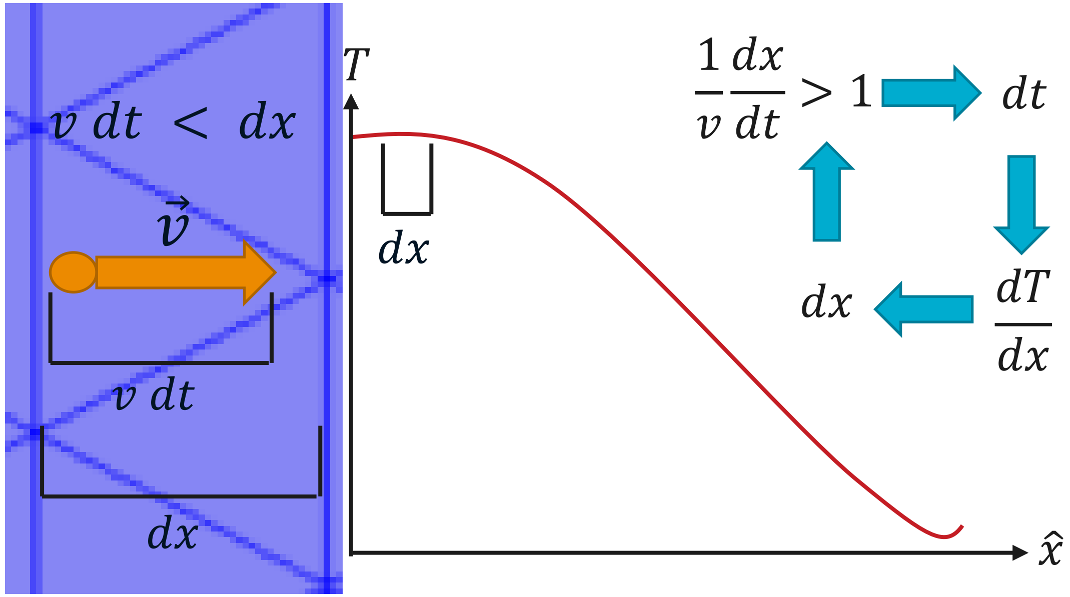

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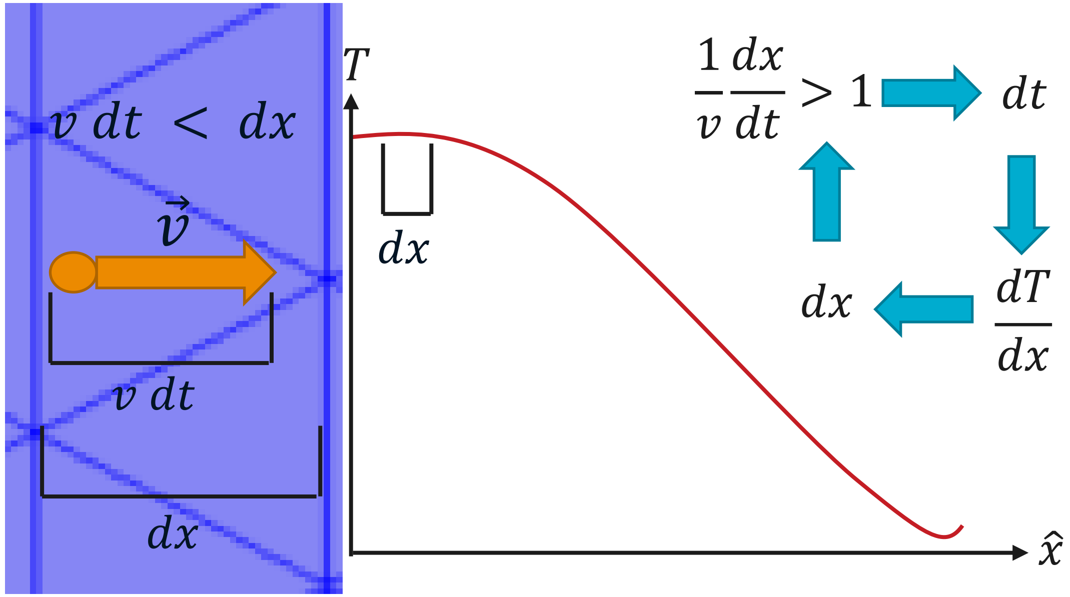

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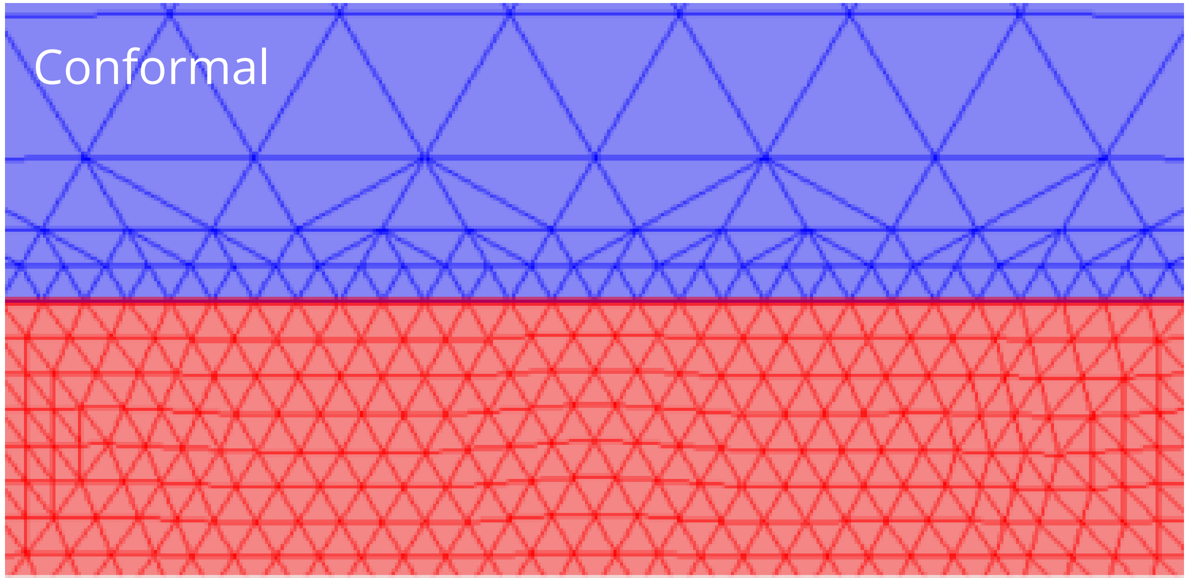
- *Conflicting simulation constraints result in unnecessarily over-constrained meshing in the plasma and time-stepping in the solid.*

- Here, we present <u>an algorithm for decoupling the spatial discretizations</u> in finite element PIC simulations, as demonstrated in the Aleph code.

NON-CONFORMAL MESHES DECOUPLE DISCRETIZATION CONSTRAINTS BY DUPLICATING BOUNDARIES.

- Conformal mesh (CM) requires an interface to use the same nodes and surface elements (left).



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- Conformal mesh (CM) requires an interface to use the same nodes and surface elements (left).
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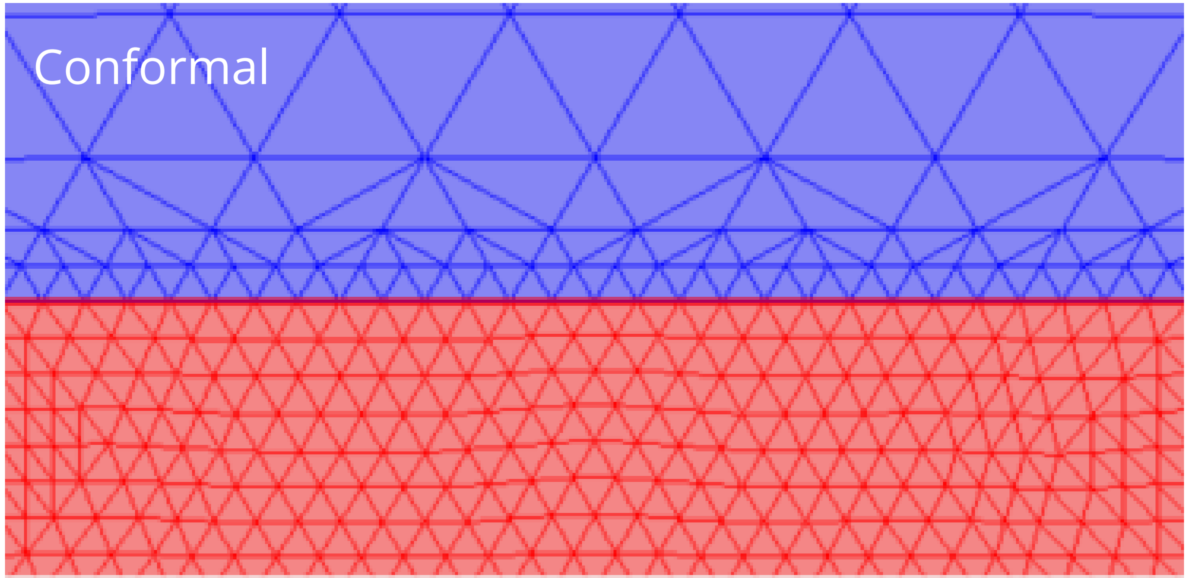

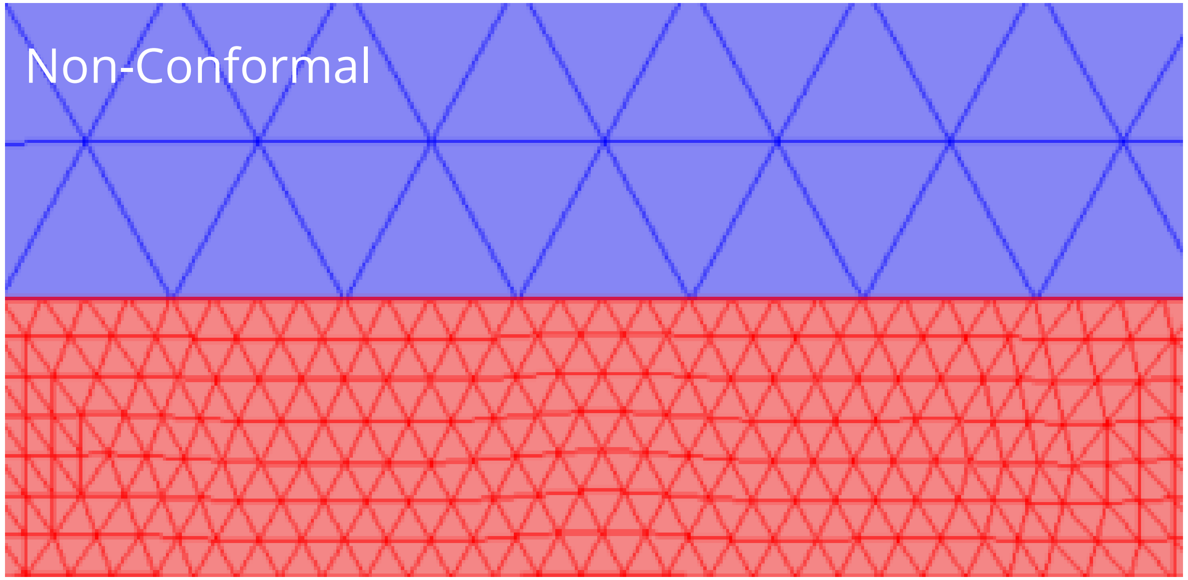

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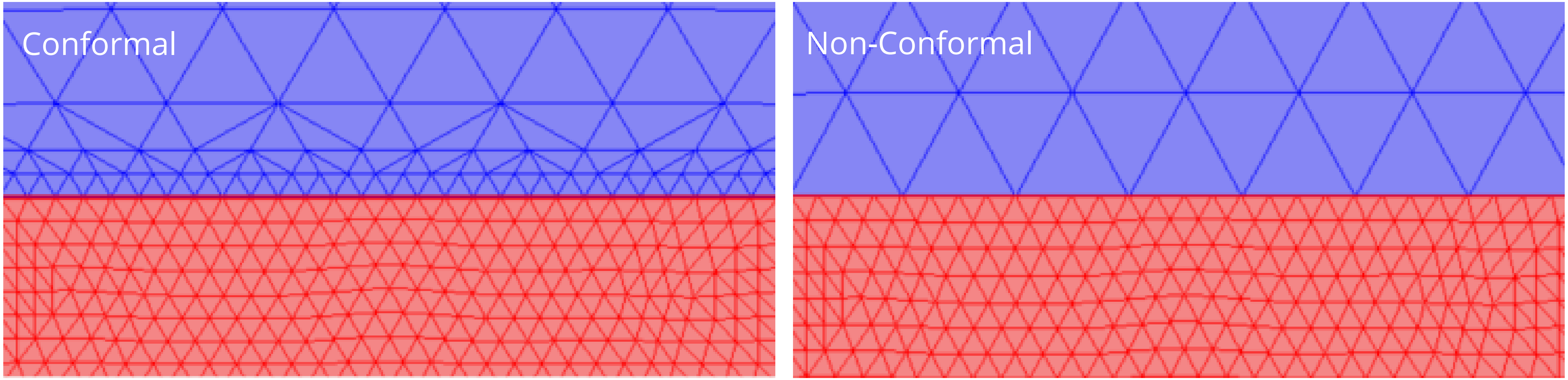
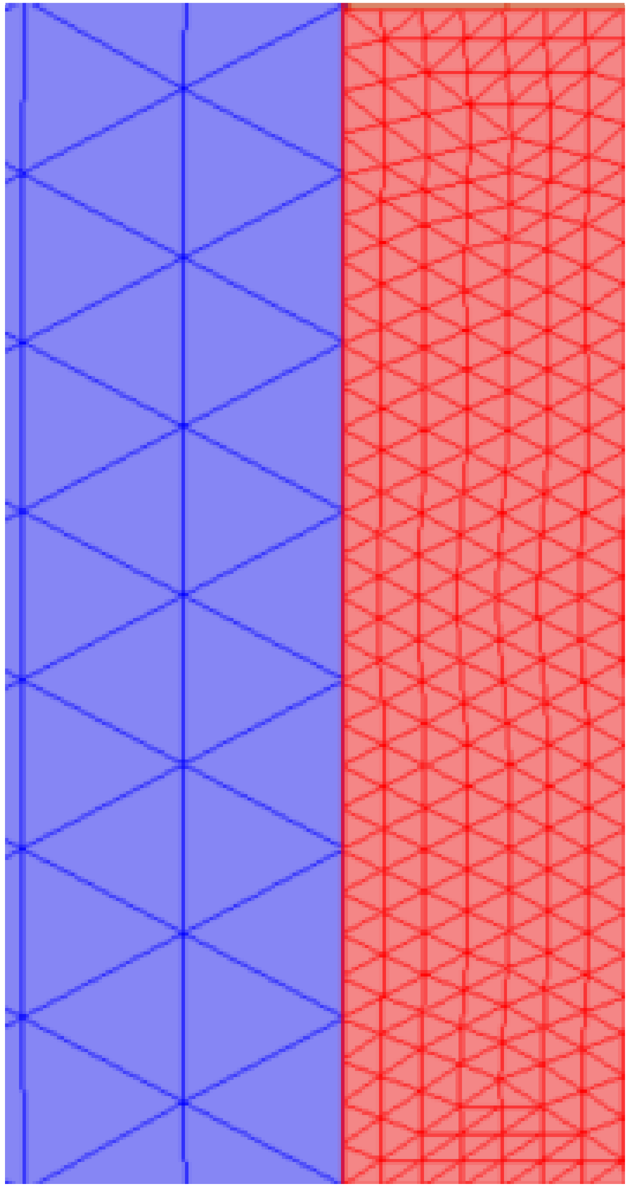
- Conformal mesh (CM) requires an interface to use the same nodes and surface elements (left).
- Non-conformal mesh (NCM) interfaces contain two sets of nodes/elements (right) which may not be co-located and therefore may result in interpolated information across the interface.
- Differing discretizations in each domain are thereby decoupled (no mesh grading necessary).
- An algorithm to map between these sets is required for proper information transfer.



AN ALGORITHM FOR MAPPING AND INFORMATION TRANSFER ACROSS NON-CONFORMAL INTERFACES:



- Algorithm links elements on one surface to elements on the other surface of the NCM interface to transfer information between.
- Three categories of mapping: one-to-one (black), many-to-one (green, left arrow), and one-to-many (light blue, right arrow).

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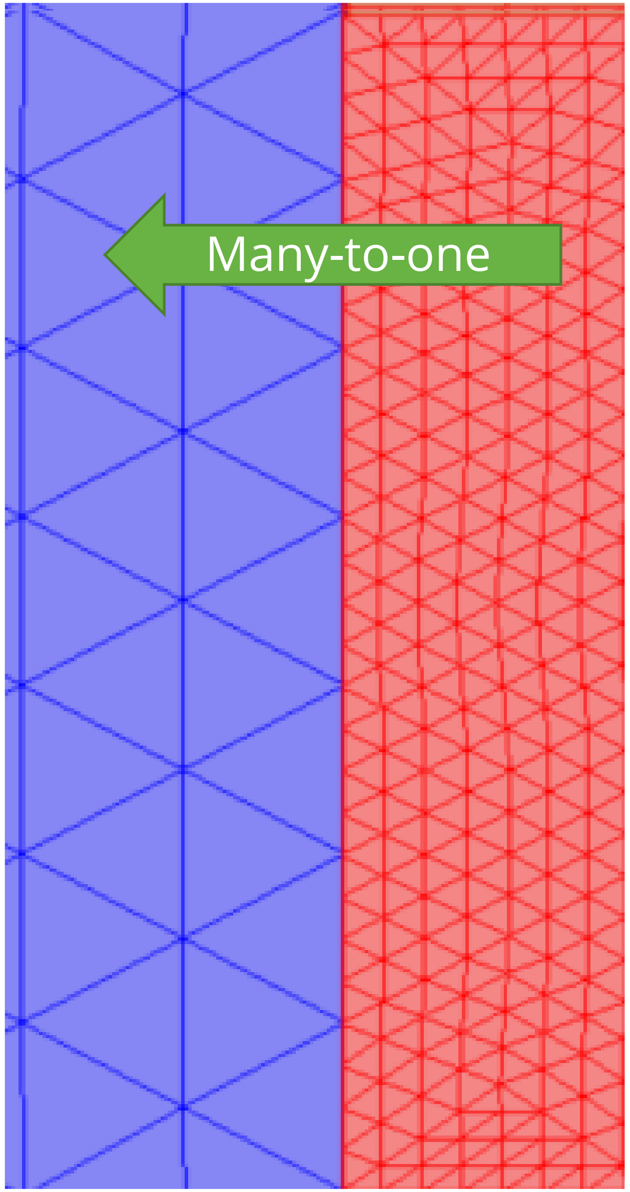

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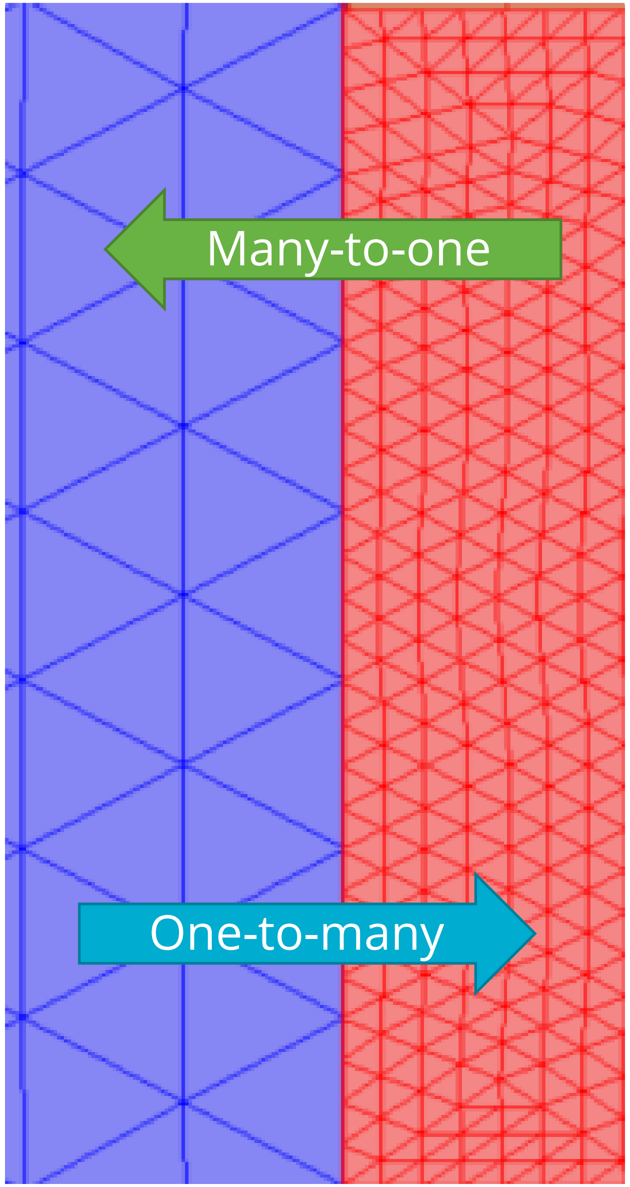

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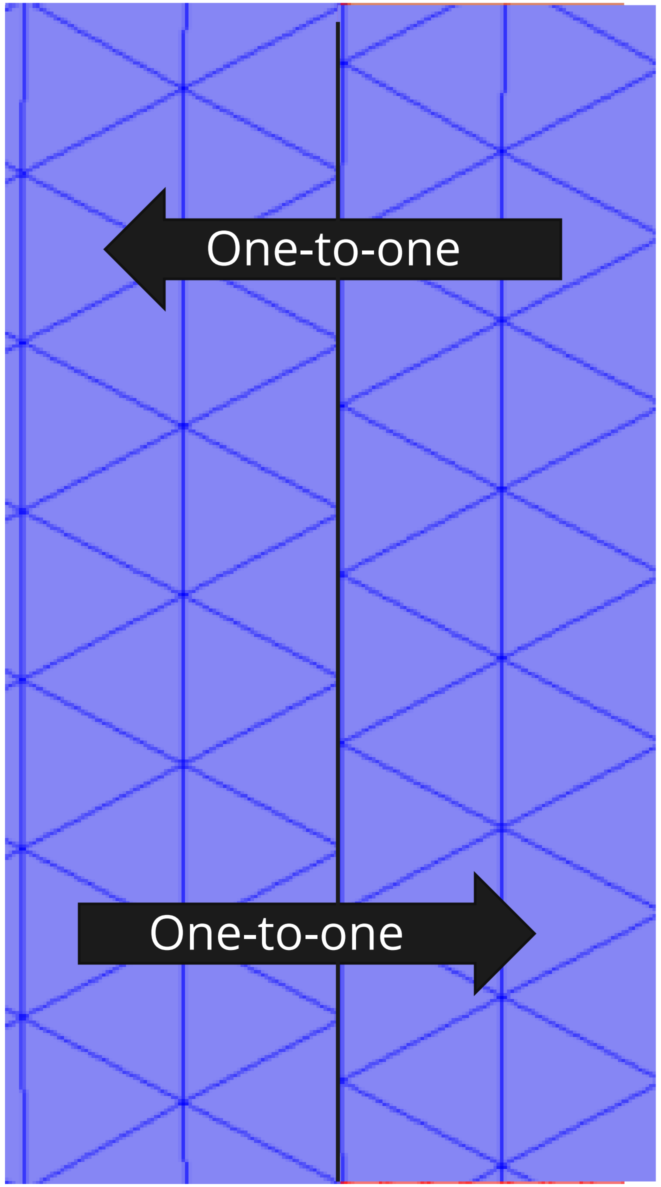

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- One-to-many maps a single element of a coarser mesh onto numerous elements of a finer mesh, splitting the associated information between them.
- One-to-one mapping only implies single element to single element correlation and does not necessarily imply co-located nodes or similar surface elements.
- Numerous caveats can complicate these mappings (e.g., discretized curved surfaces, “smearing”).

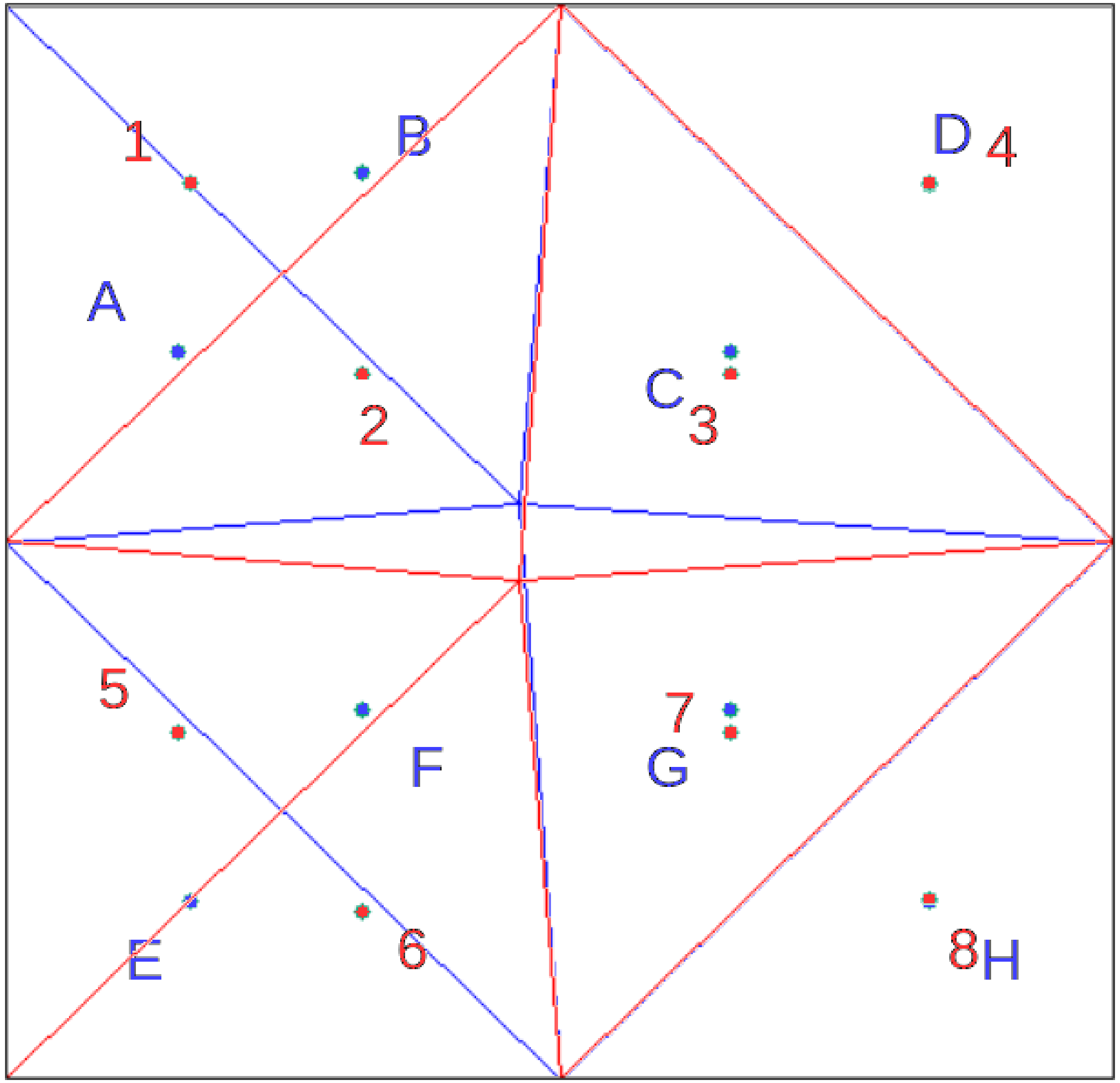
AN ALGORITHM FOR MAPPING AND INFORMATION TRANSFER ACROSS NON-CONFORMAL INTERFACES:

- A pre-processing step maps two surfaces of a non-conformal interface by projecting the centroids of source (red, numbers) surface elements onto destination (blue, letters) elements and vice versa.

- When more than one centroid maps to one element, the source information (S_{ei}) is collated in a weighted sum, where f_i is the fraction of S_{ei} to transfer:

$$D_e = \sum_i f_i S_{ei} \quad (1)$$

- $f_i = 1$ (one-to-one, many-to-one) or $f_i = 1/N_D < 1$ (one-to-many), where N_D is number of destination elements for that source element.



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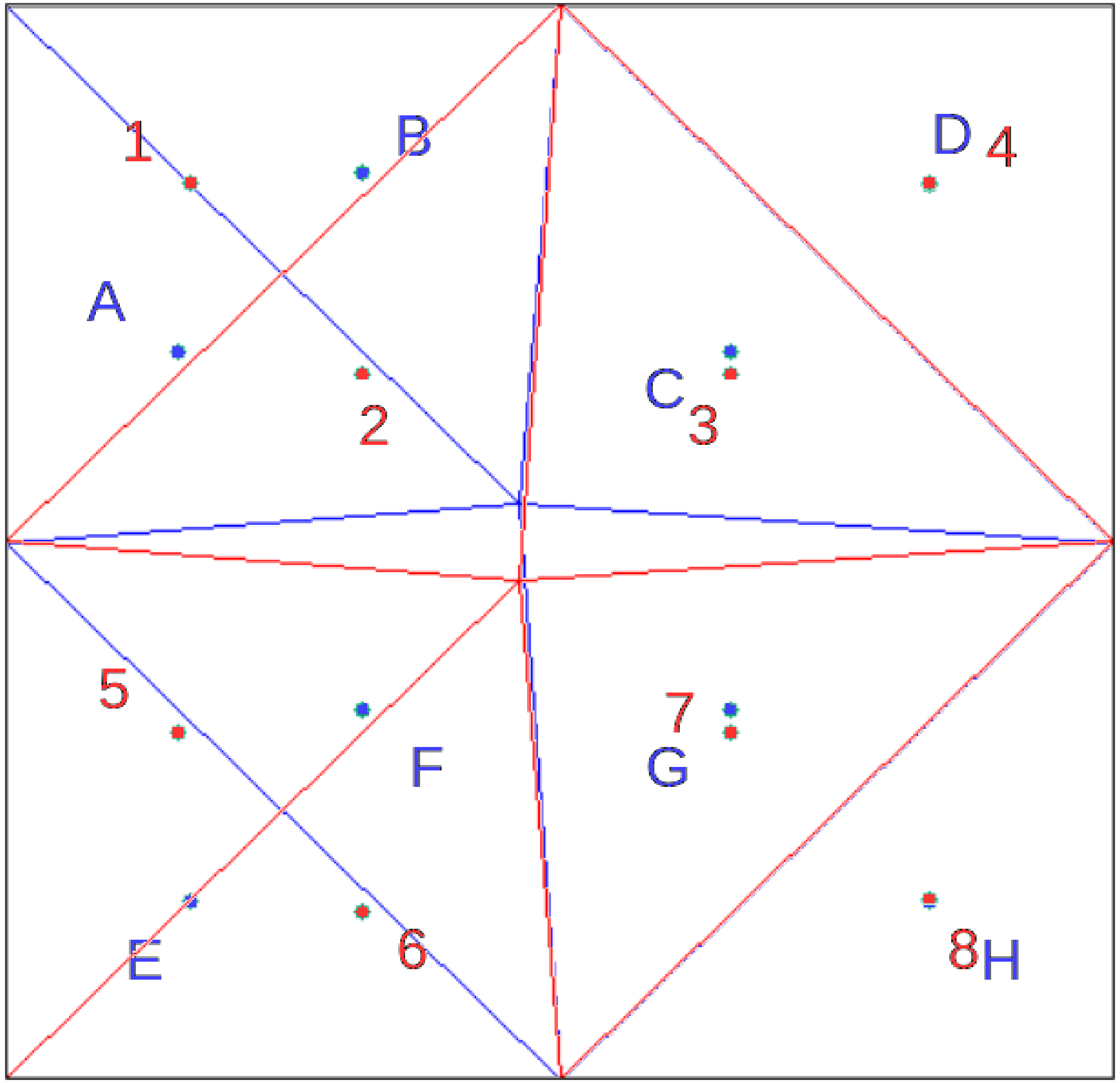
Source Elements	Destination Elements
3	C
4	D
7	G
8	H



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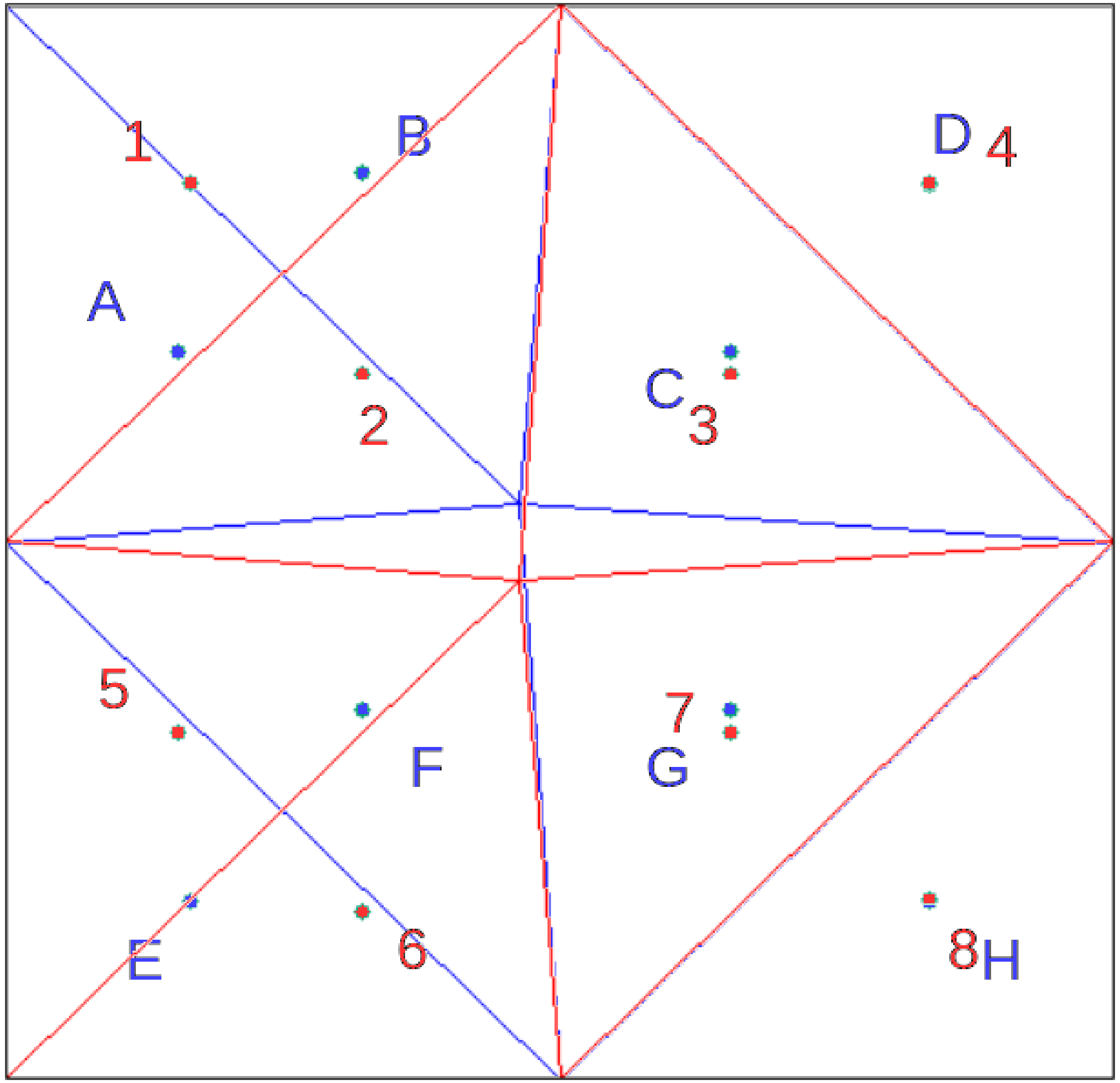
Source Elements	Destination Elements
	A
	B
	E
	F

- Two passes of mapping are required:



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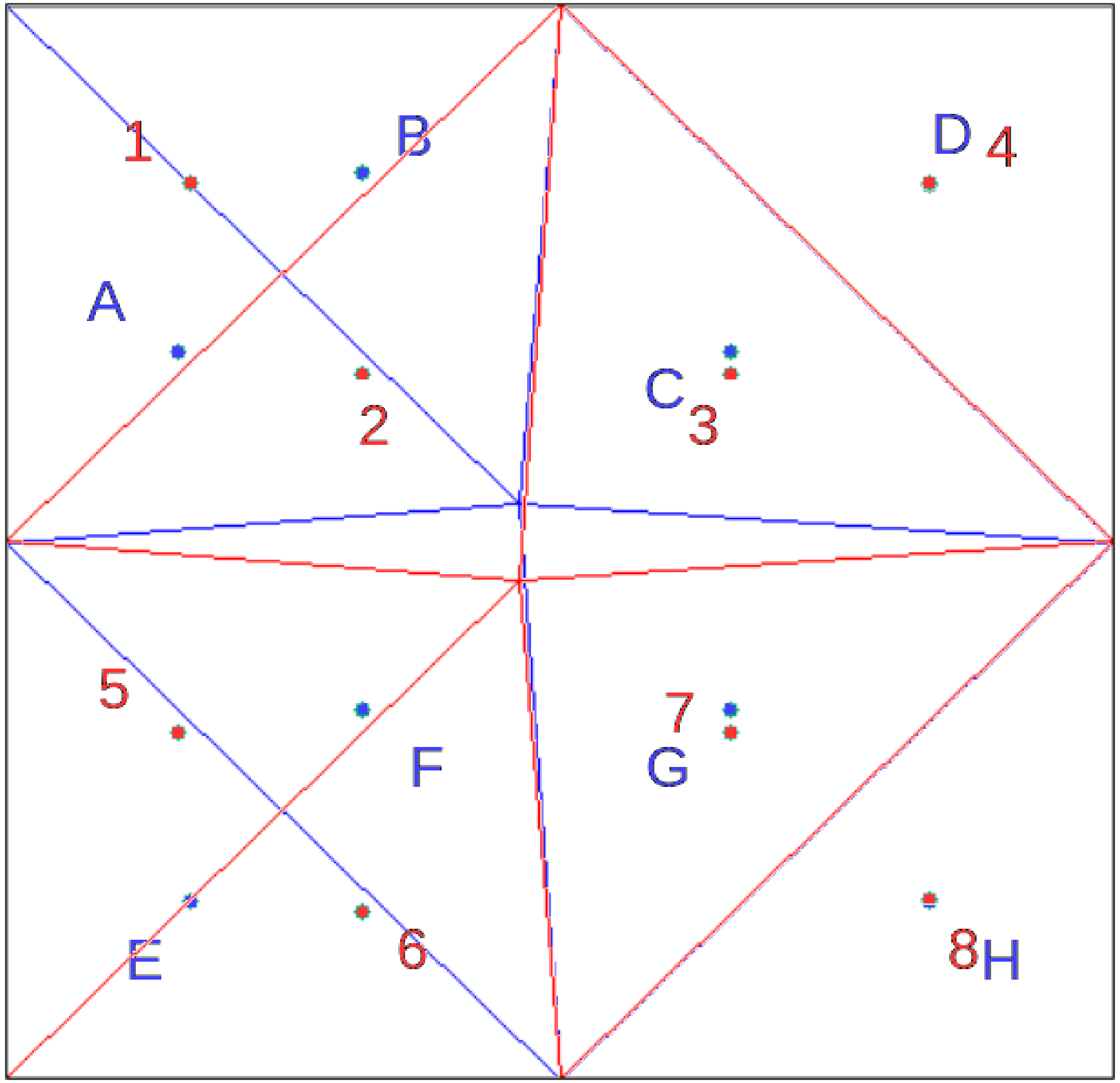
Source Elements	Destination Elements
1	A
1	B
? (5 or 6)	E
5	F

- Two passes of mapping are required:
  - Destination to source association.



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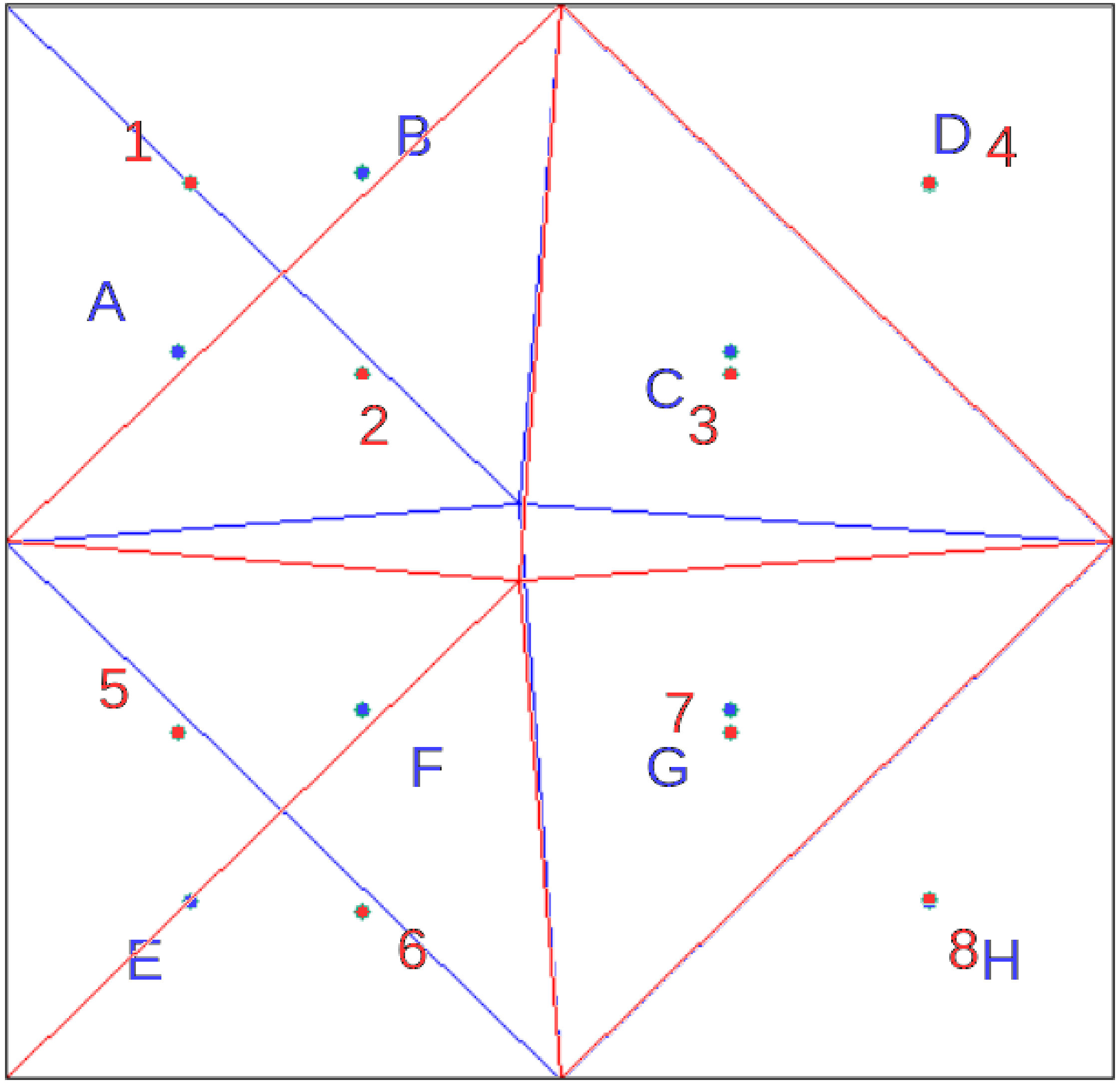
- A pre-processing step maps two surfaces of a non-conformal interface by projecting the centroids of source (red, numbers) surface elements onto destination (blue, letters) elements and vice versa.

Source Elements	Destination Elements
1, 2	A
1	B
? (5 or 6)	E
5	F

- Two passes of mapping are required:
  - Destination to source association.
  - Source to destination association (deals with unassociated elements, e.g. 2).



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Source Elements	Destination Elements
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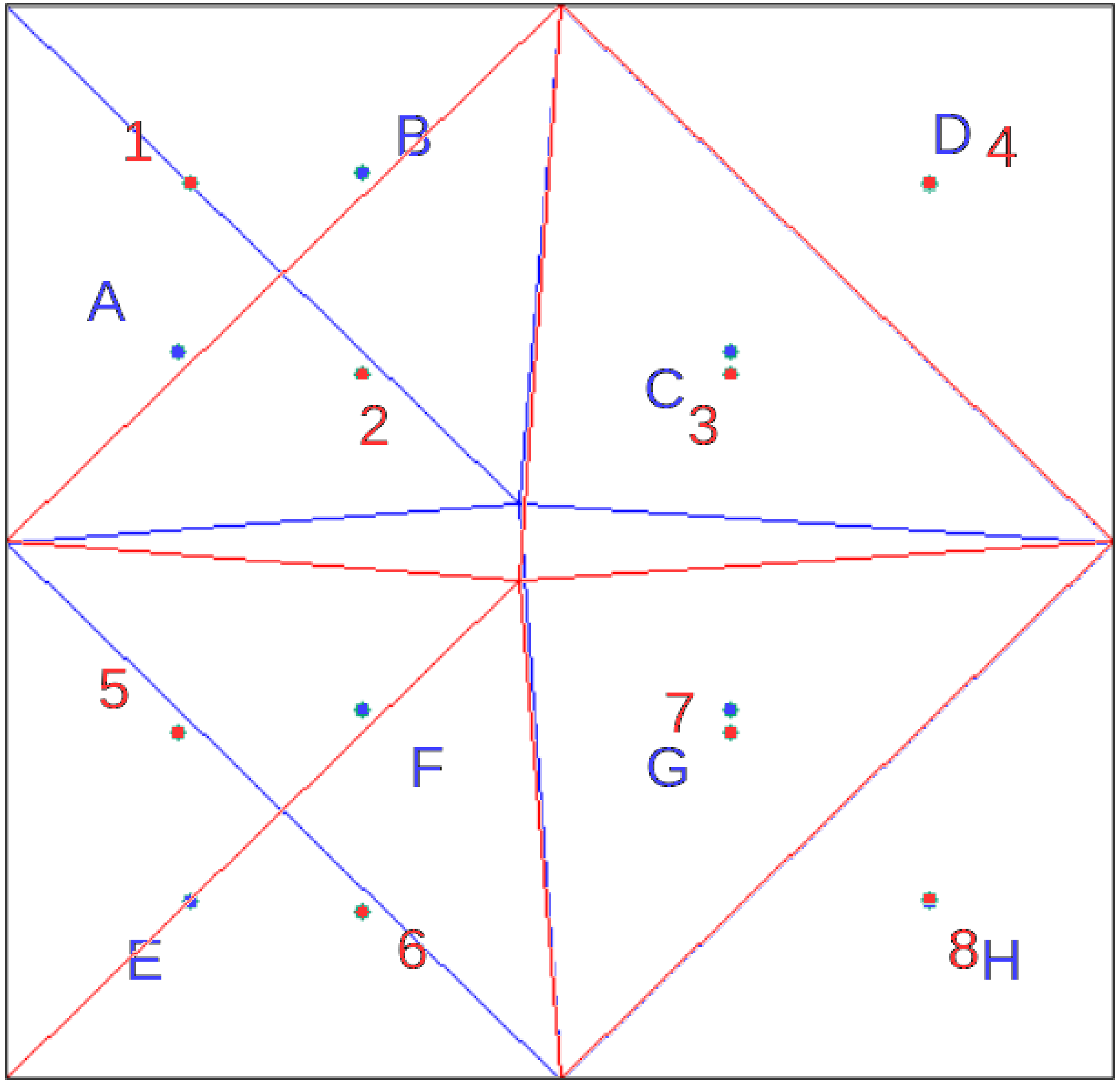
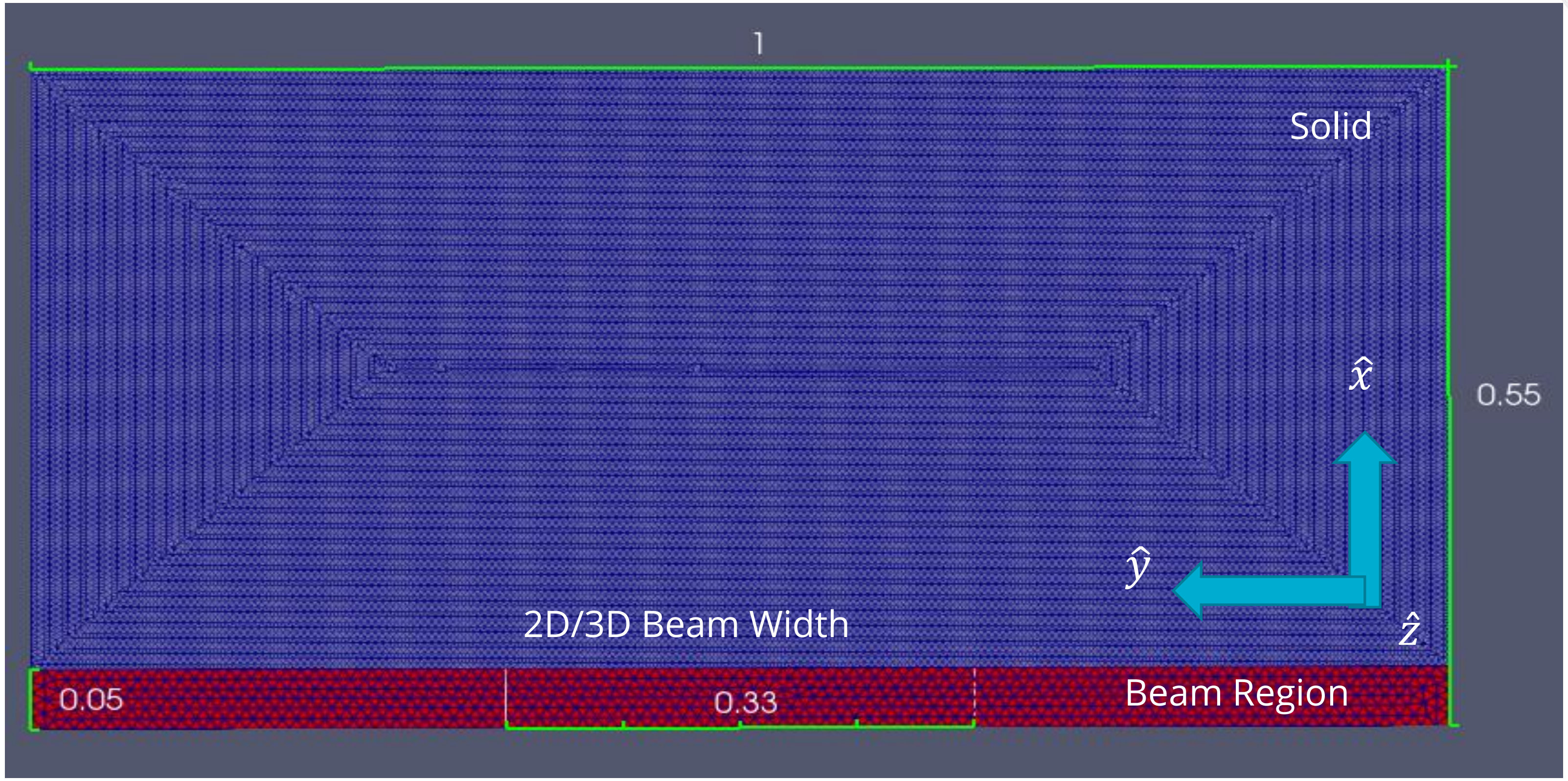
6	E
5	F

- If a centroid lands on the border of two elements (see centroid E), a tie-breaker selects one source element, prioritizing those with no associated destination (element 6).



ALEPH PIC SIMULATIONS OF PARTICLE BEAM HEATING SOLID INTERROGATES THE EFFICACY OF INFORMATION TRANSFER.

Beam Region Discretization dx (m) for NCM	Solid Discretization dx (m) for both CM and NCM
0.01	0.01
0.01	5.0e-3
0.01	2.5e-3
0.01	1.25e-3
0.01	6.25e-4
0.01	3.125e-4
0.01	1.5625e-4



Heat equation: $\frac{\partial T}{\partial t} = \alpha \nabla^2 T$ (2)

$\alpha = k/\rho C_p = 1.0$ = thermal diffusivity

$k = 1.0$ = thermal conductivity

$C_p = 1.0$ = solid specific heat

- Solid material properties and particle beam heat flux (q_s) are set such that $T(t = 0.1\ s, x = 0.0\ m) = 2.0\ K$ for a 1D analytic solution with $T_i = 1.0\ K$ into the solid ($\hat{x}$ direction):

$$T(t,x) = T_i + \frac{2q_s\sqrt{\frac{\alpha t}{\pi}}}{k} e^{\left(\frac{-x^2}{4\alpha t}\right)} - \frac{q_s x}{k} \operatorname{erfc}\left(\frac{x}{2\sqrt{\alpha t}}\right) \quad (3).$$ [1]

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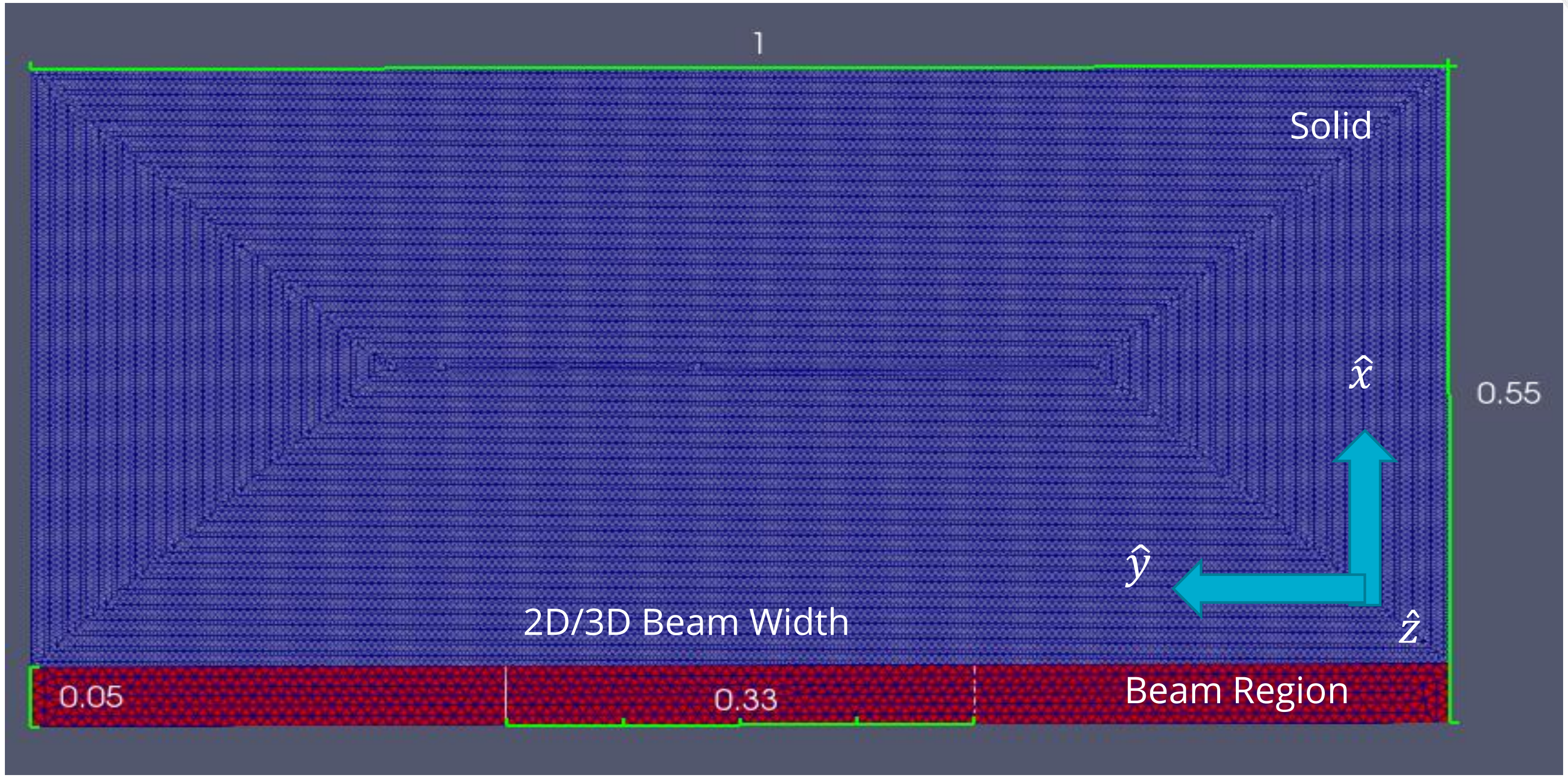
In conformal meshes, beam region and solid discretizations are identical.

In non-conformal, the beam region retains the largest discretization (as above).



- In quasi-1D, a 2D geometry is used but beam covers the solid surface. 2D/3D examines lateral heat conduction using a fixed beam width.
- Emission of identical particles confirms solid to beam region information transfer (but with no associated heat loss) with the flux:

$$\phi_{emit} = \frac{10^{-1/T}}{\sqrt{2\pi k_B T}} \quad (4).$$

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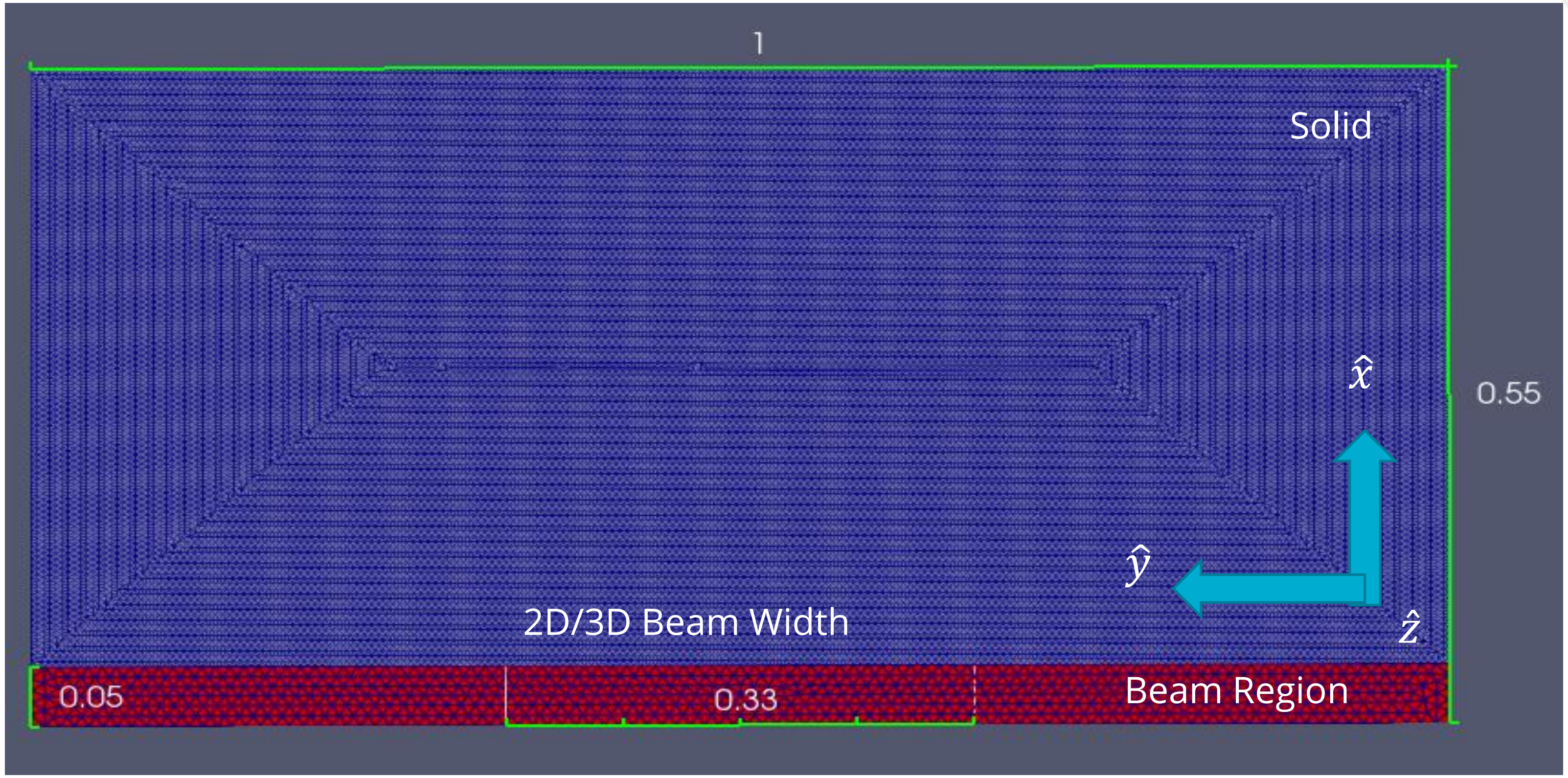


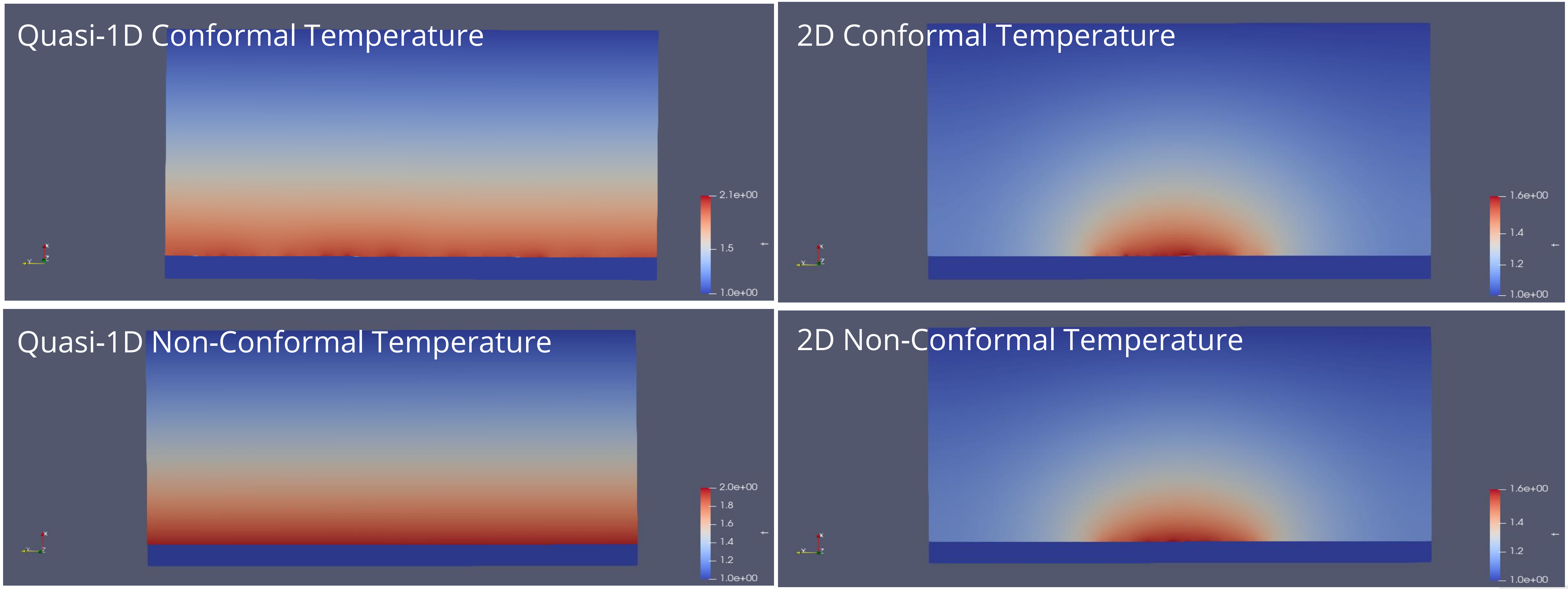
In conformal meshes, beam region and solid discretizations are identical.

In non-conformal, the beam region retains the largest discretization (as above).

- The CFL condition is intentionally ignored to achieve highly refined meshes. Particle dynamics do not affect particle collection at the surface and electric fields are not included (neutral particles).
- The timestep constraint from the solid thermal solve is used instead.
- Beam particles traverse the plasma gap in one timestep (with intentionally fixed velocity) and impart a fixed heat flux (q_s) by moderating the particle mass and numeric particle flux.

SIMULATIONS DEMONSTRATE NON-CONFORMAL INFORMATION TRANSFER DOES NOT CHANGE MULTIPHYSICS.

- The particle beam similarly heats the solid in both CM and NCM (dx=1.5625e-4 m shown).
- The lateral heat conduction in 2D/3D reduces max surface temperature (1.6 K vs 2.0 K in 1D).



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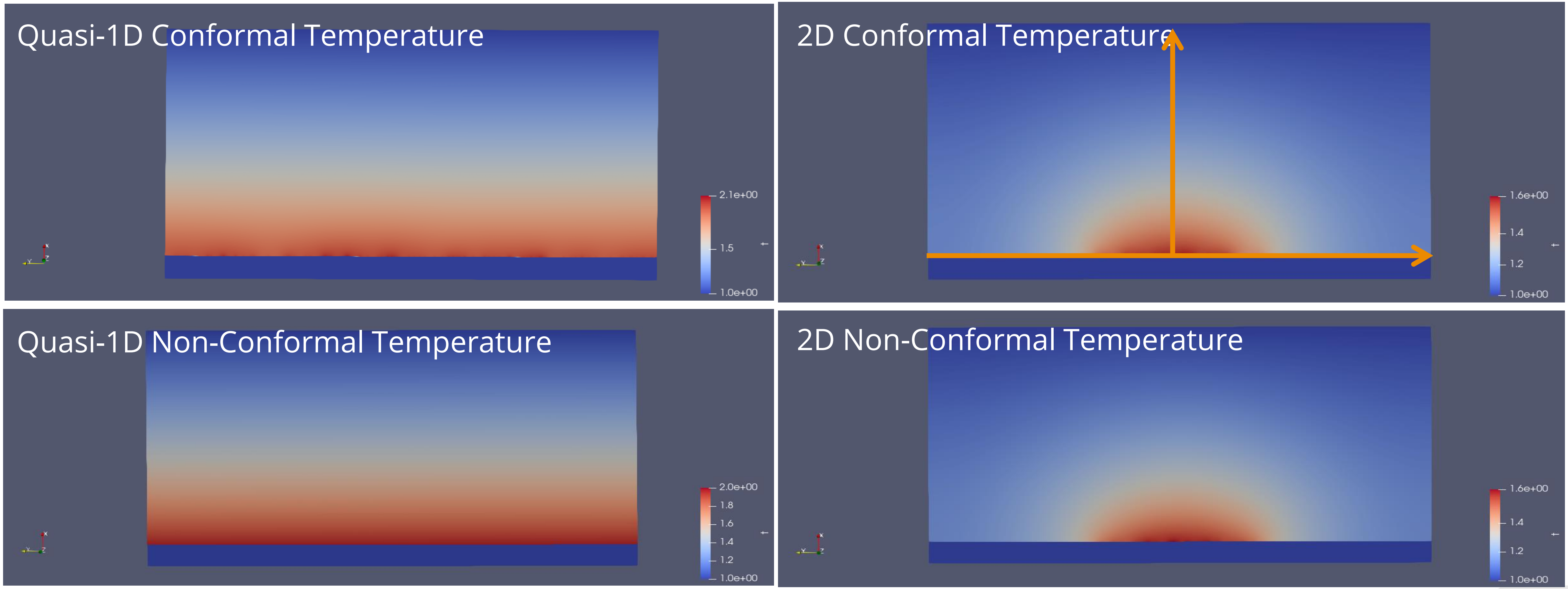
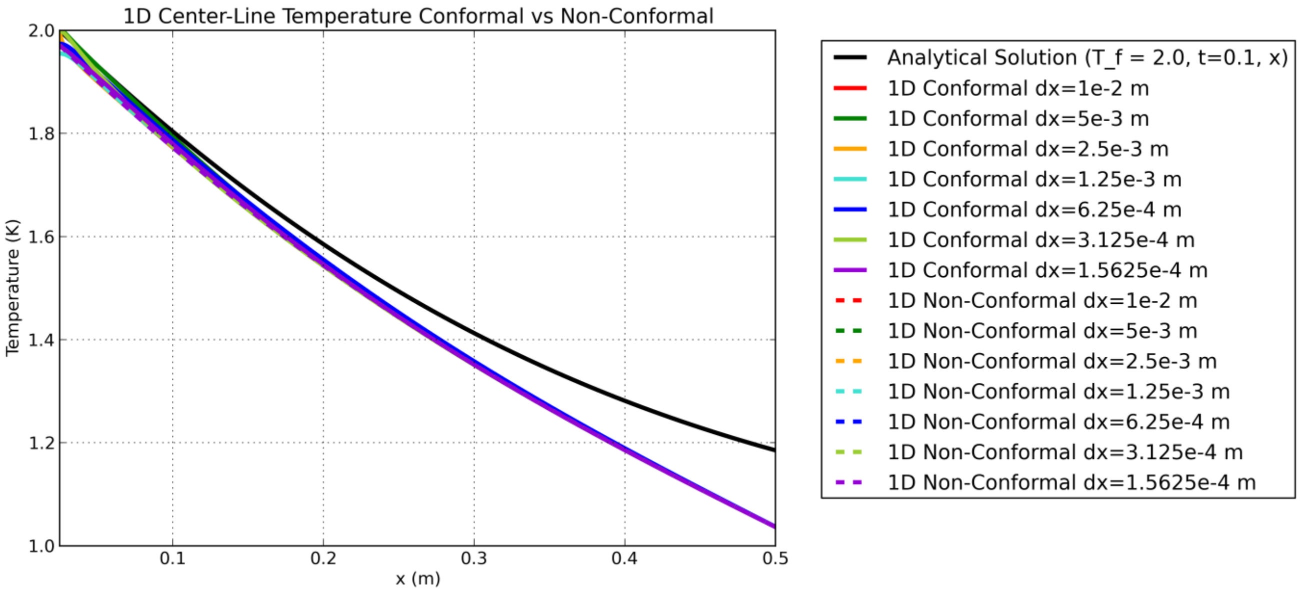
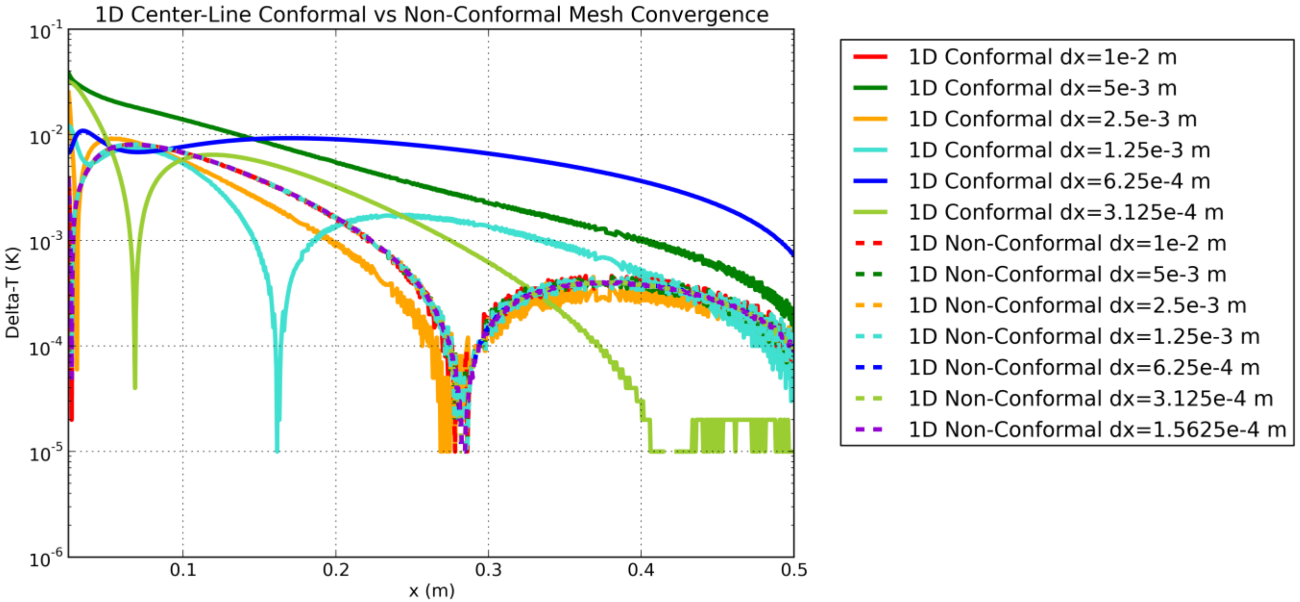


COMPARISON OF CONFORMAL AND NONCONFORMAL SIMULATIONS SHOWS IDENTICAL CONVERGENCE BEHAVIOR.

- In 1D, we compare to the analytic solution in a semi-infinite slab of eqn. (3) (upper plot, black line).
- Discrepancy between analytic solution and other curves is due to the small domain (in x) and a Dirichlet boundary condition of $T = 1$ K.
- Delta-T compares to the finest conformal mesh case.
- *The decoupling algorithm does not affect convergence behavior between CM and NCM.*





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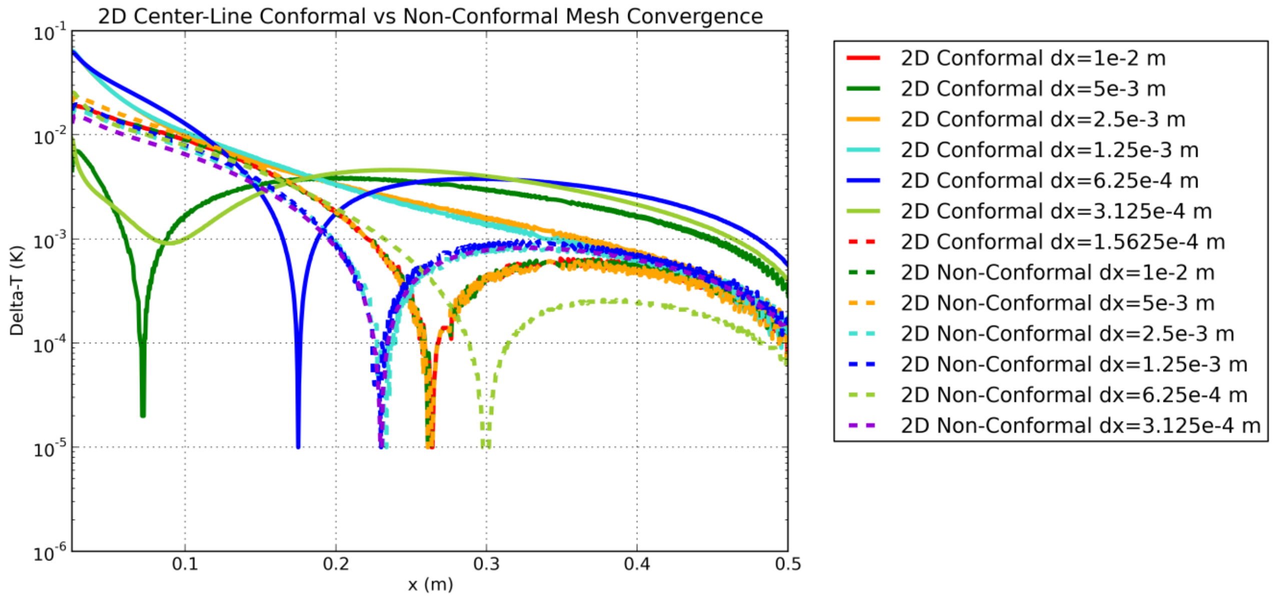
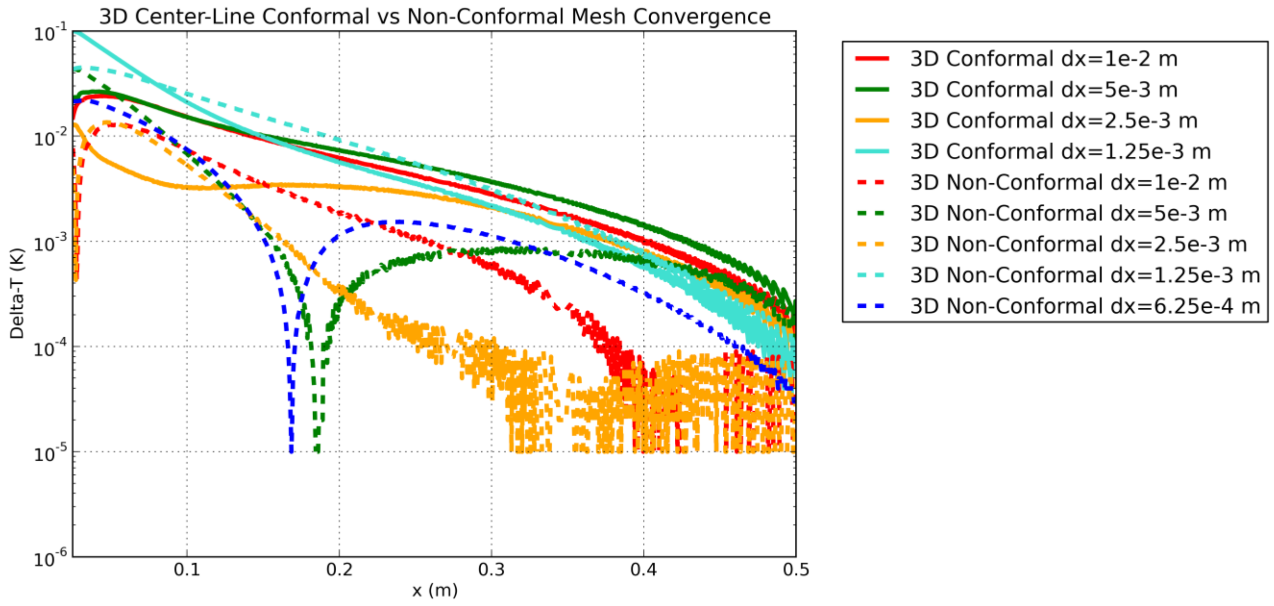
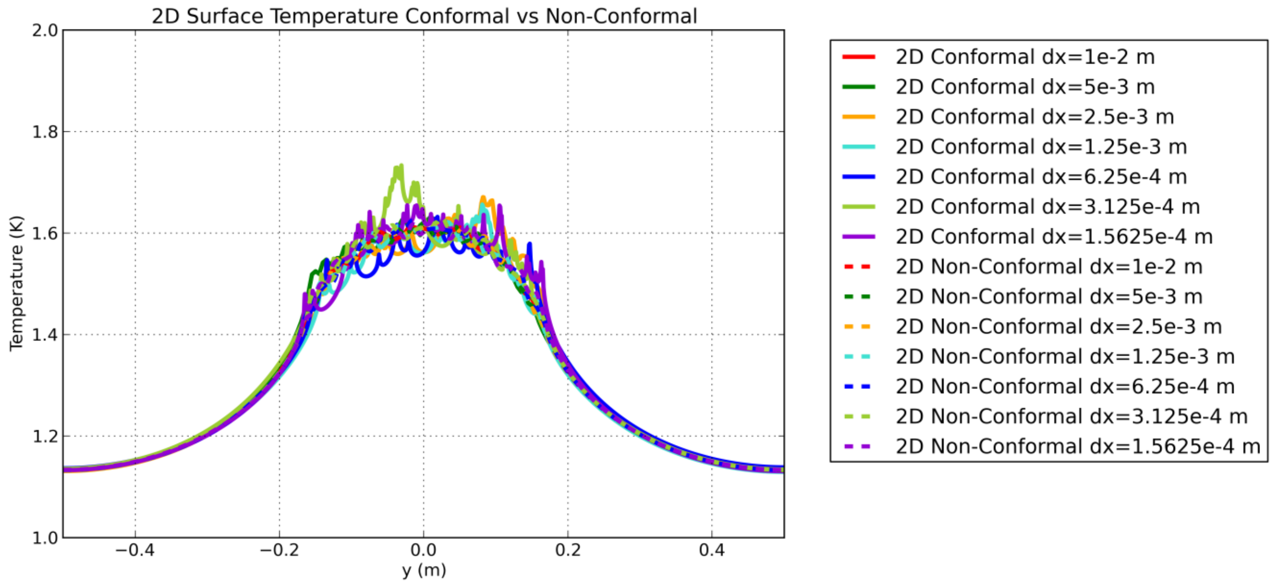
- Delta-T compares to the finest conformal mesh case.
- *The decoupling algorithm does not affect convergence behavior between CM and NCM.*
- Discrepancies in Delta-T are due to under-resolved particle statistics introducing hot spots and thereby noise in the surface temperature.

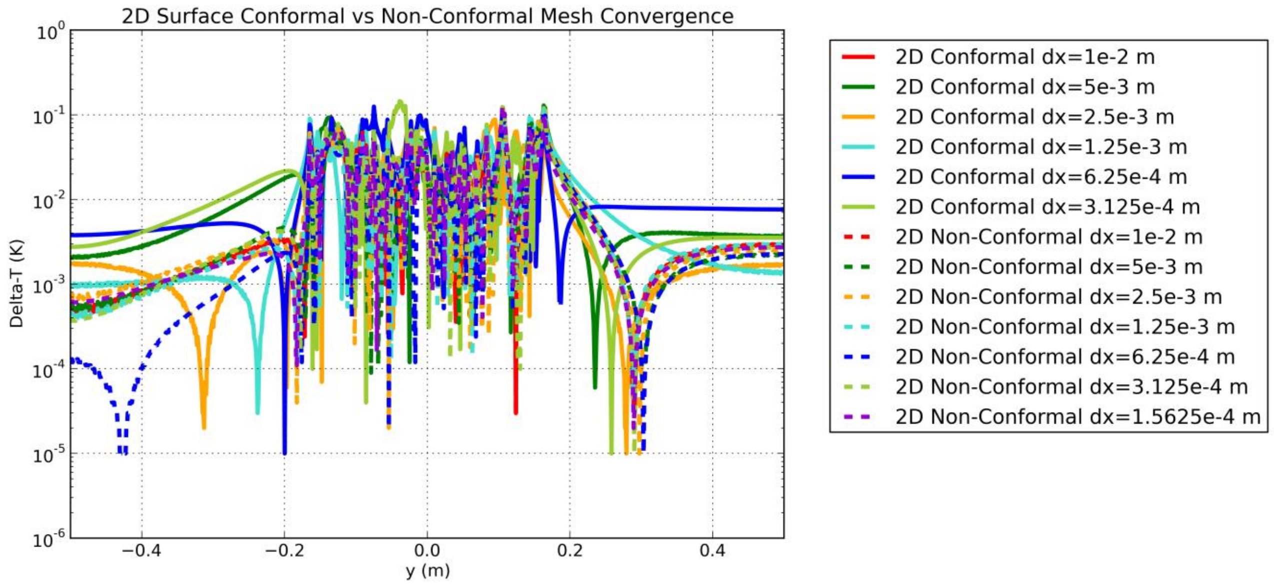




LATERAL HEAT CONDUCTION BETWEEN CONFORMAL AND NONCONFORMAL CASES BEHAVES SIMILARLY.

- Delta-T compares to the finest conformal mesh case.
- Lateral heat conduction behaves identically in the regions outside where the beam heats the solid.
- Non-physical "hot spots" occur where the beam particles hit in both CM and NCM. Tuning mass and numeric flux or smoothing algorithms addresses this.





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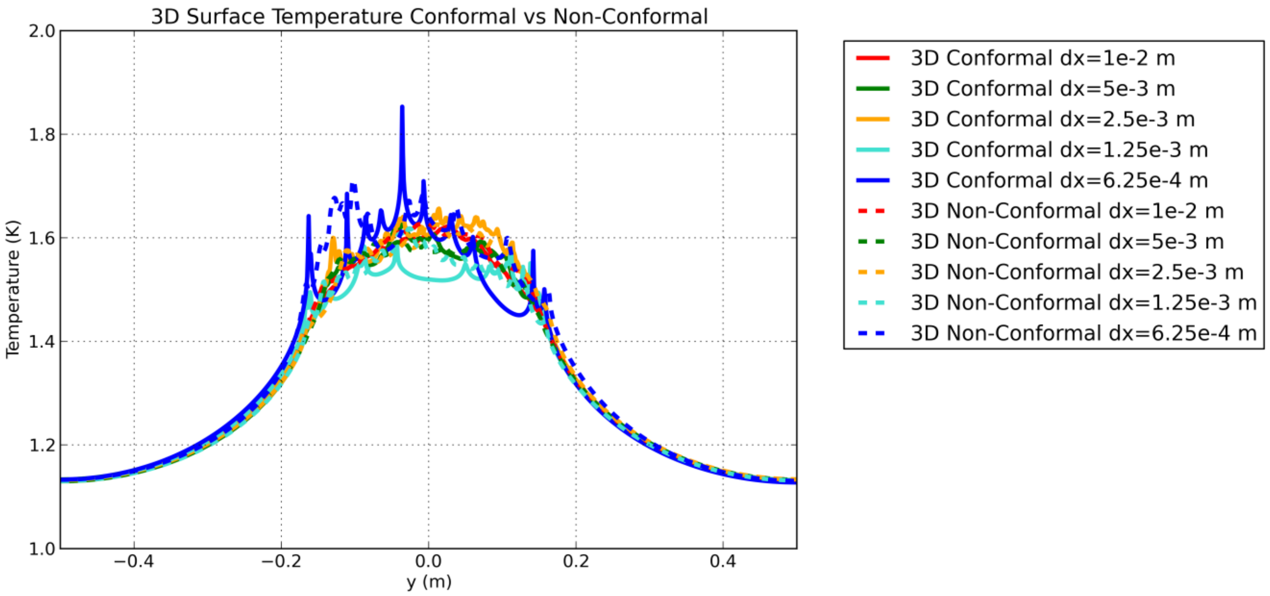
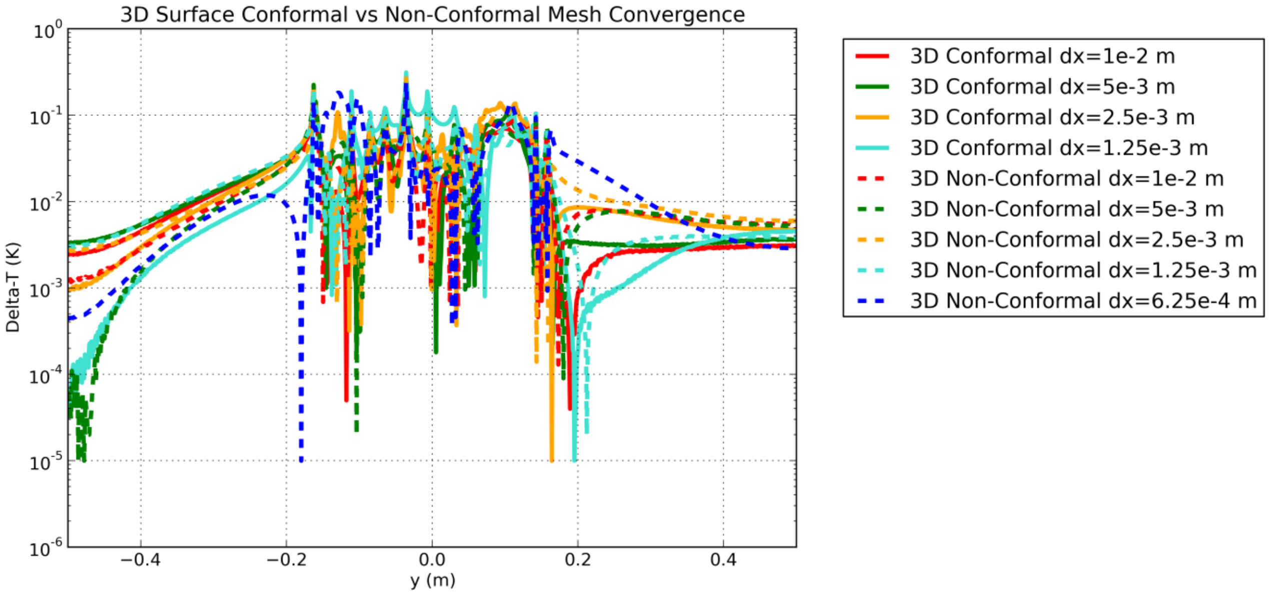
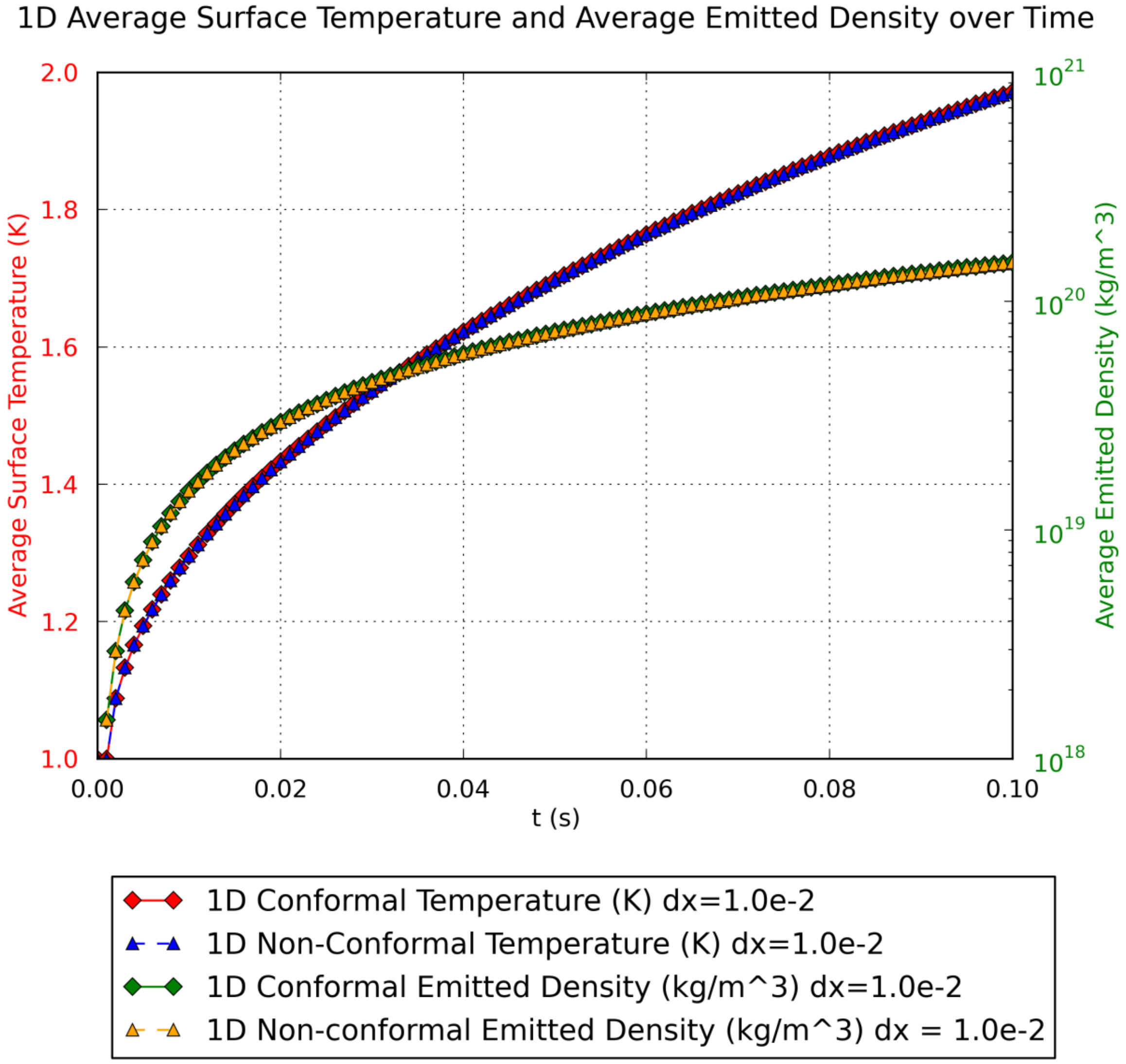
- Lateral heat conduction behaves identically in the regions outside where the beam heats the solid.
- Non-physical “hot spots” occur where the beam particles hit in both CM and NCM.
- Hot spots exacerbated in 3D due to increased surface areas and under-resolved particle statistics.





PARTICLE EMISSION CONFIRMS INFORMATION TRANSFER IN OPPOSING DIRECTION (SOLID TO BEAM REGION).

- Particle emission changes non-linearly due to the increasing temperature of the emitting surface.



Averages are over the surface lineout.

NONCONFORMAL CASES SHOW AN IMPROVEMENT IN SIMULATION EFFICACY.

- *Speedup of several orders of magnitude is observed in "real" simulations due to orders of magnitude difference in mesh element size (discretization) causing several effects:*
    1. E.g., <u>A 400x improvement in timestep</u> due to 400-1 mesh element size ratio.
    2. <u>Fewer elements</u> involved in certain field solvers (e.g., electric potential).
    3. <u>Fewer total superparticles</u> required for accurate plasma statistics.

- Some of the above effects are not showcased here as particles traverse the beam region in one timestep and do not include other field solvers. The primary effect, here, is not over-meshing the beam region (effect 2 above).

- <u>Some constraints may still play a role in limiting the overall timestep (dt)</u> (effect 1) without including sub-cycling/super-cycling of timesteps (e.g., upper limits on stability).

CONCLUSIONS

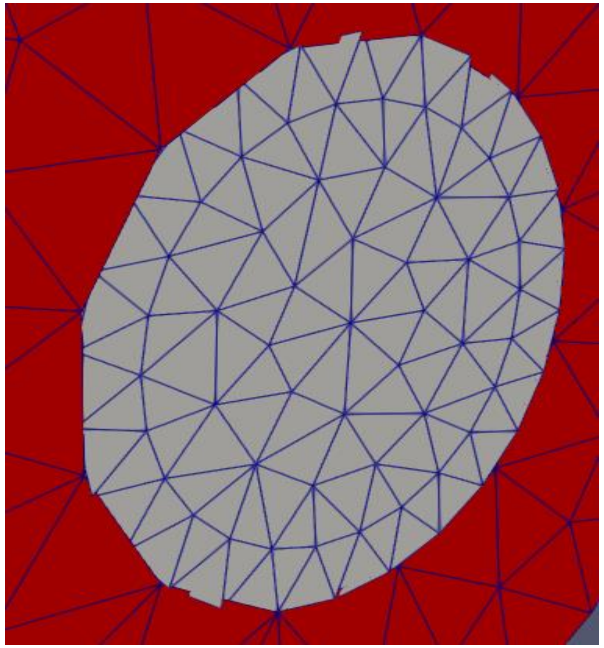
- An algorithm for decoupling spatial discretizations in multiphysics PIC simulations was developed and tested for a simplified simulation of a particle beam heating a solid.

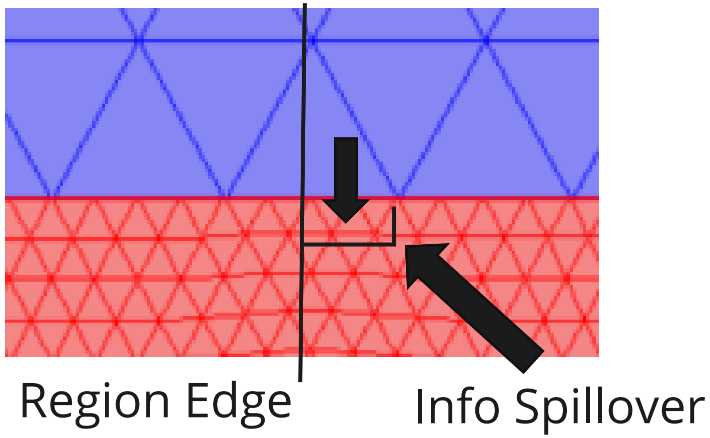
- This algorithm utilizes a pre-processing stage that maps one surface of a non-conformal interface onto the other and vice versa.

- *Comparisons of the conformal (traditional information transfer) and non-conformal (using the new algorithm for information transfer) mesh cases demonstrate the correctness and accuracy of this algorithm while enabling a significant reduction in mesh complexity.*

- This non-conformal mesh capability therefore leads to improvements in the efficacy of running complicated multiphysics simulations where vastly differing spatial discretizations are necessary or desired.

FUTURE WORK WILL FURTHER IMPROVE SIMULATION EFFICACY AND ADDRESS CURRENT CAVEATS.





- <u>Timestep super-cycling, Semi-Implicit PIC (SIPIC [2]), and NCMs together optimize certain PIC simulations</u> of plasmas and improve iteration speed for a variety of applications.
- Non-conformal interface mapping works in parallel, but initial mapping has memory limitations for finer/complicated meshes. Every processor related to interface needs a copy of the mapping.
- Smoothing algorithms or time-averaging provide a more physical simulation without increasing particle count (alleviates “hot spots”).
- *Numerous caveats complicate this algorithm’s mappings, such as:*
  - <u>Discretized curved surfaces may not have geometric conformity and thus require more extensive interpolation</u> (top).
  - <u>Spatial “smearing” occurs from spillover of information transfer to edge elements</u> which extend beyond an intended recipient region (bottom).

QUESTIONS?

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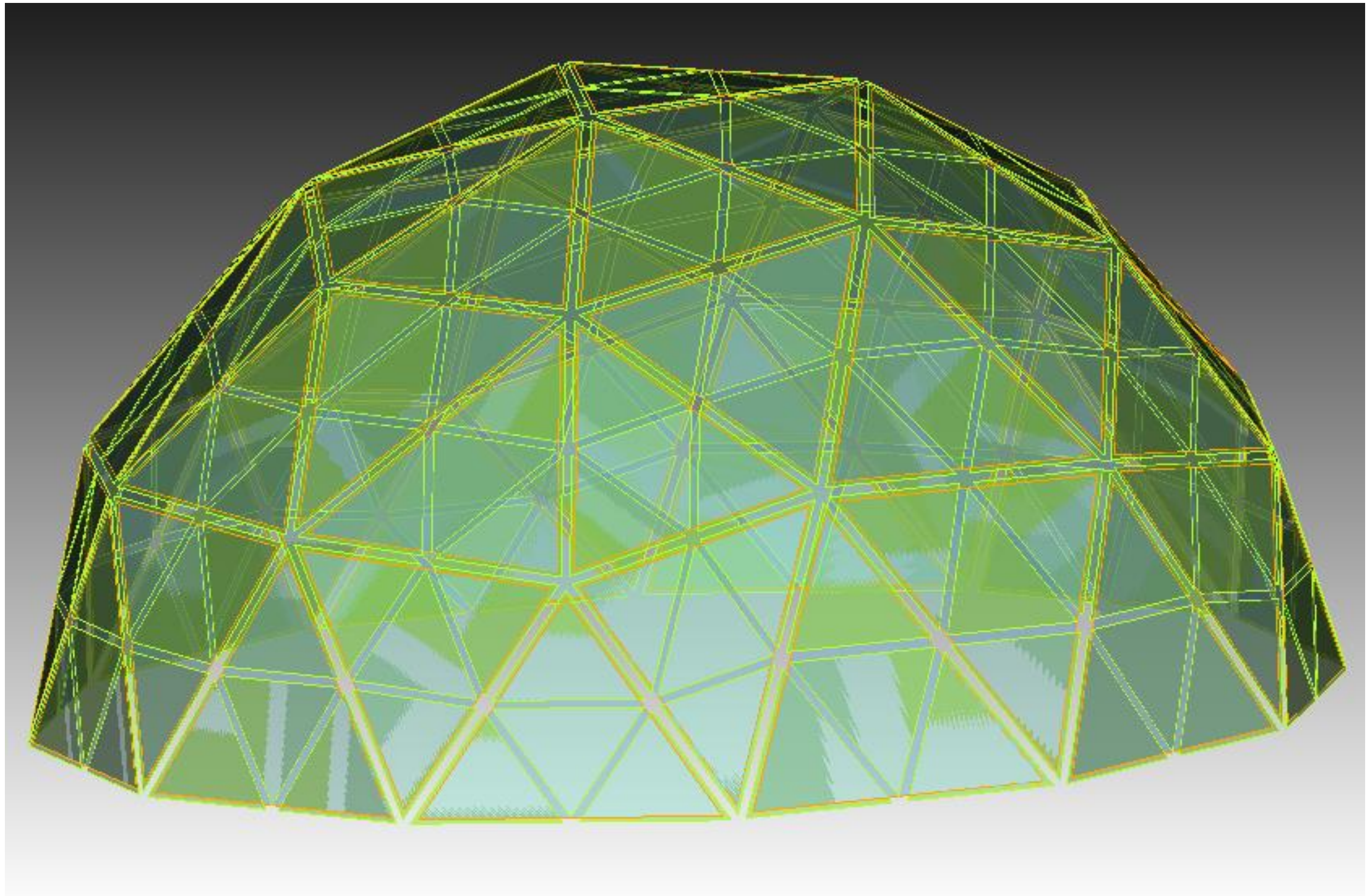
[1] R. Hooper and S. Moore, “Aleph Field Solver Challenge Problem Results Summary”, Technical Report, Sandia National Laboratories, Jan. 2015

[2] D. C. Barnes, “Improved C1 shape functions for simplex meshes”, J. Comp. Phys, 424, 109852, 2021.

BACKUP: CAREFUL MESHING OF DISCRETIZED CURVED SURFACES ALLEVIATES GEOMETRIC OVERLAP



- Geometric conformity can be preserved on discretized curved surfaces with differing dx, but only if the coarse geometry is maintained on the finer mesh.
- *Therefore, geometric conformity (linear interfaces) without mesh conformity (i.e., a NCM) is possible.*
- Removes the additional interpolation considerations from geometric overlap that typically occurs for NCM curved interfaces.
- Requires mesh refinement of the fine domain after initial meshing of the coarse mesh geometry.