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Automatic Coarsening of the Particle Interaction Mesh in a Hybrid PIC-DSMC Simulation

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Introduction

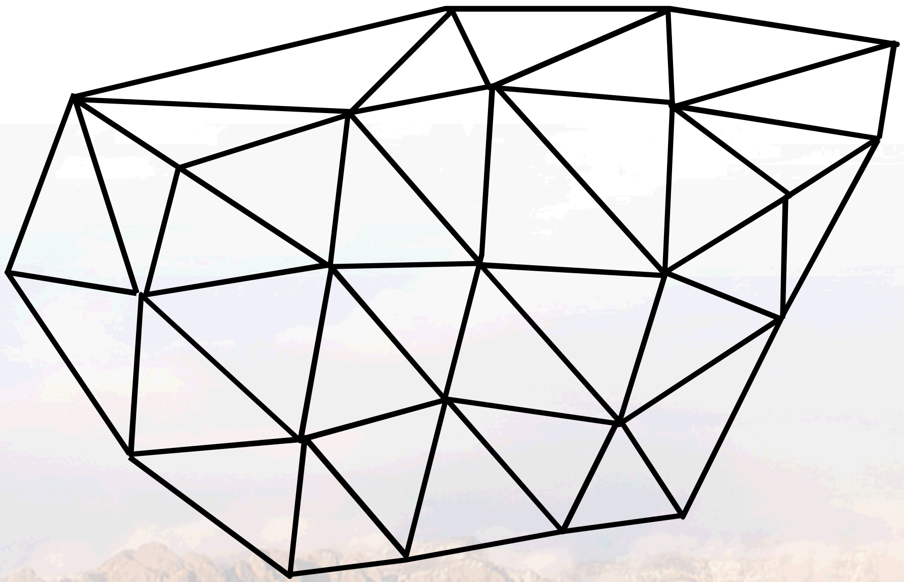
- Hybrid particle-in-cell (PIC) and direct simulation Monte Carlo (DSMC) methods are frequently used to simulate low density interacting plasmas
- A single mesh is often used for both PIC and DSMC calculations
- The mesh size for PIC is often limited by the Debye length
- The collision cell size for DSMC is limited by the mean free path (can be much larger than the Debye length)
- Too few computational particles per DSMC collision cell can lead to errors
- Therefore, the optimal PIC mesh may be suboptimal for calculating DSMC collisions

Overview of New Patching Method

- Use a fine mesh for PIC (unstructured)
- Use a rectangular grid to conglomerate many PIC elements into a single DSMC collision cell
- Size DSMC collision cells based on mean free path, λ_{mfp}
- Use oct-tree algorithm to adjust the size of DSMC collision cells on the fly

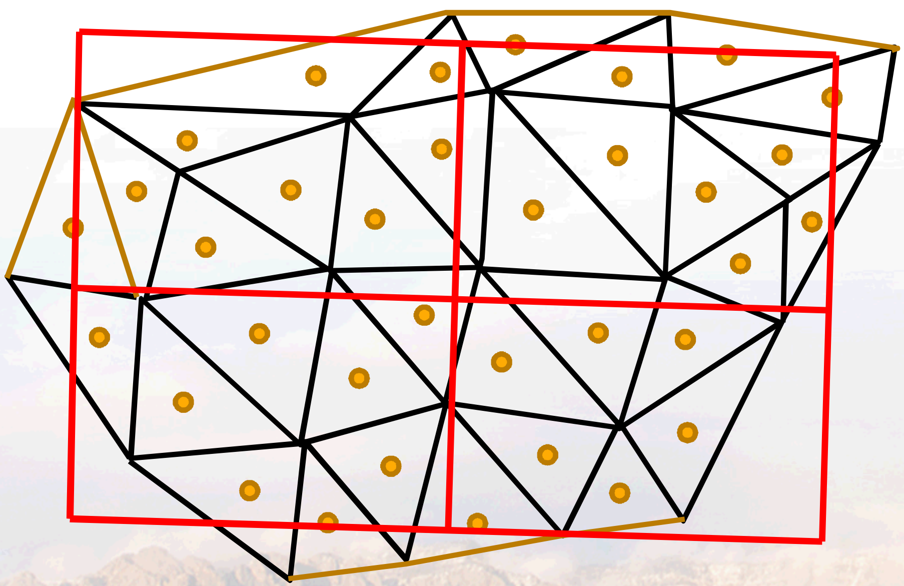
Patch Method

- **Original (unstructured) PIC mesh**



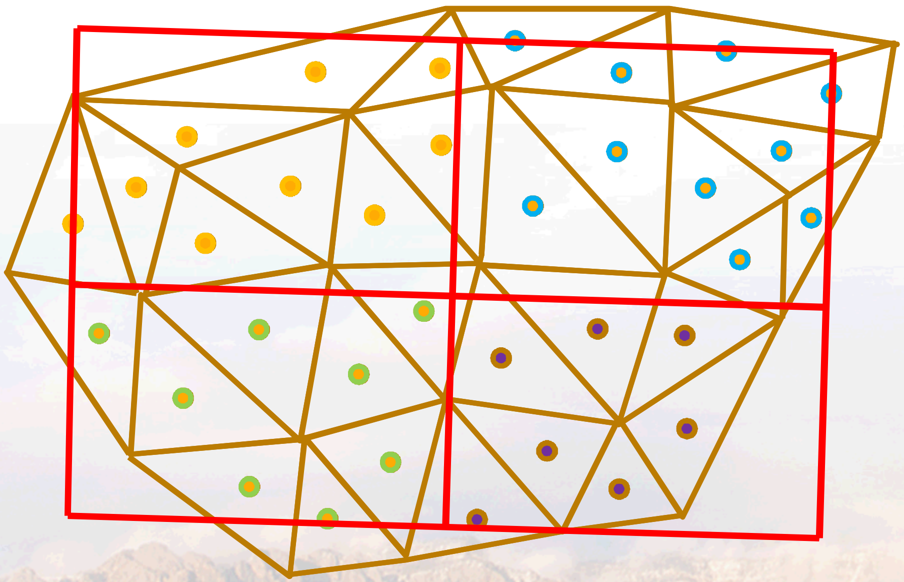
Patch Method

- Apply rectilinear grid based on element centroid

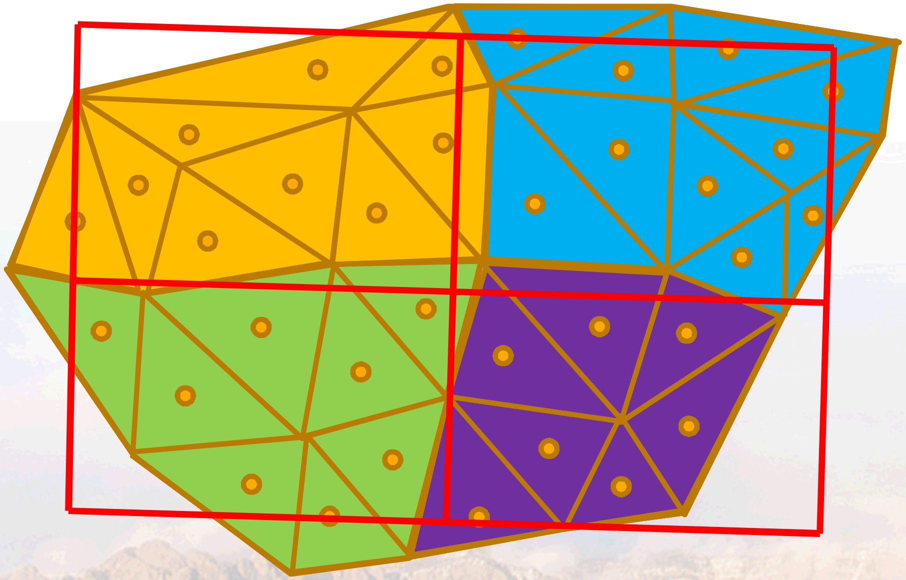


Patch Method

- Assign elements to patches (based on element centroid)



Patch Method

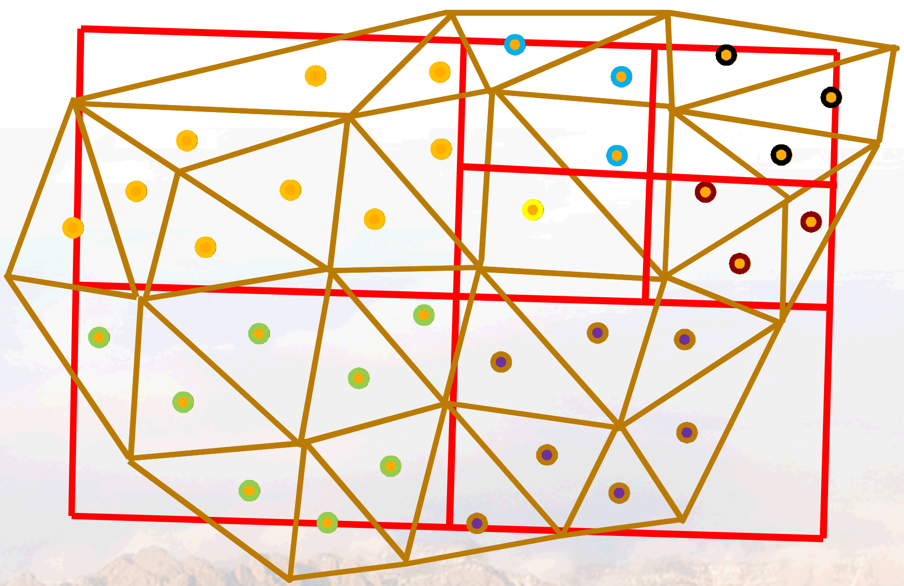


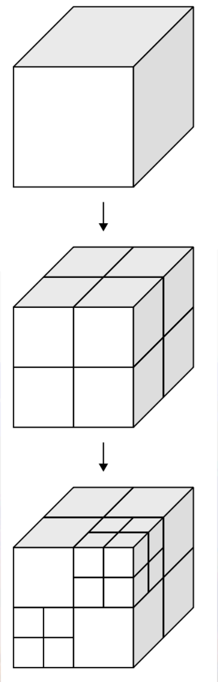
Patch Method

- Patched mesh
- Use patches to compute DSMC collisions

Oct-tree Refinement

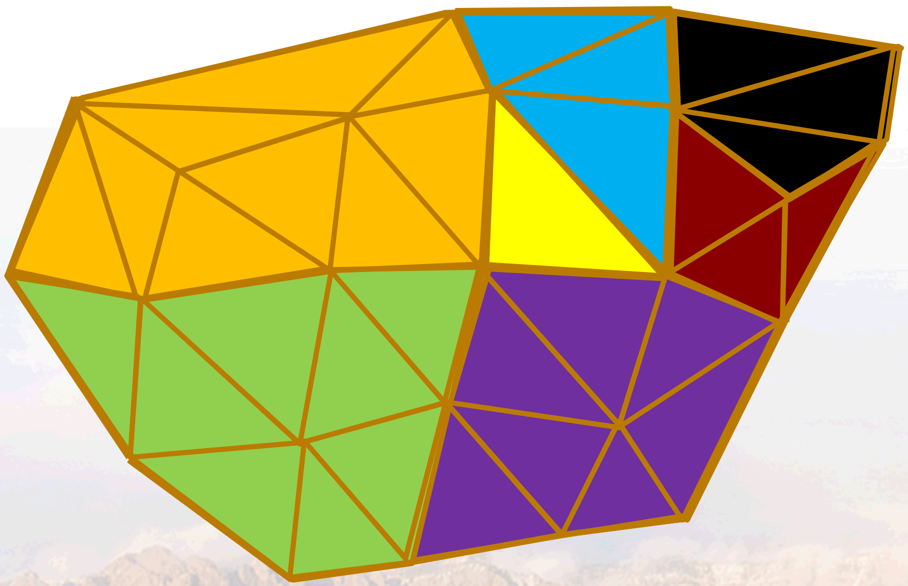
- Use oct-tree algorithm to refine mesh based on mean free path





Oct-tree Refinement

- Refined mesh



Automatic Sizing of Patches

Patch size is dynamically adjusted based on the local mean free path λ_{mfp}:

1. **Compute λ_{mfp} for each interaction on an elemental basis (using all species)**
2. **For each interaction, average λ_{mfp} over elements in the oct-tree cell**
3. **Take the minimum of all the average λ_{mfp} and divide by 2, use this to size patches using the oct-tree algorithm**

Temporal Averaging

- **Calculate λ_{mfp} for each element as:**

$$\lambda_{\text{mfp}} = \frac{v}{Z} n$$

v = velocity
Z = interaction frequency
n = number of particles

- **With a high computational particle weighting, temporal smoothing is needed. Can use either:**

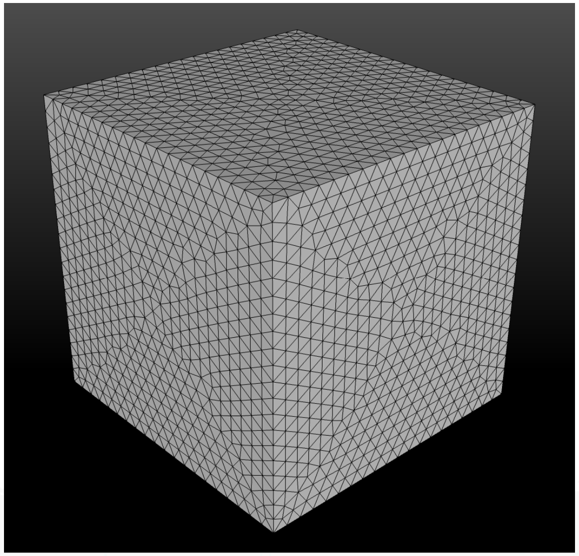
$$\langle \lambda_{\text{mfp}} \rangle = \left\langle \frac{v}{Z} n \right\rangle \qquad \langle \lambda_{\text{mfp}} \rangle = \frac{\langle v \rangle}{\langle Z \rangle} \langle n \rangle$$

- **Sometimes can get zero interactions in a timestep. With the first option, this leads to division by zero**
- **Found that the second option works much better**

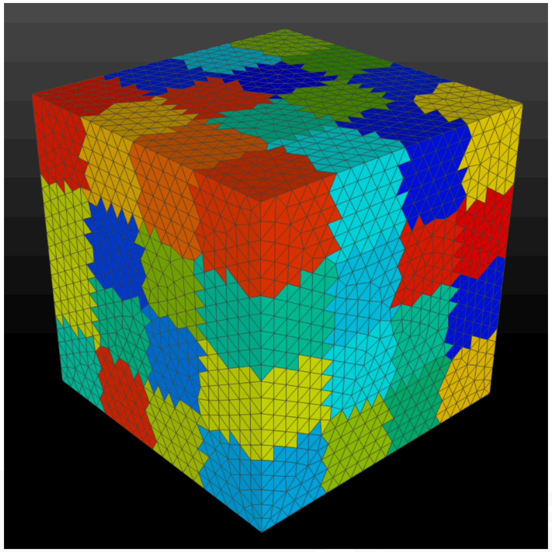
HI Test Problem

- Hydrogen iodide (HI) molecules interacting with elastic collisions
- Use variable hard sphere (VHS) interaction cross section
- T = 594.6 K, n = 10^{20} m^{-3}
- 3D cubic system, L = 5 cm
- Analytic λ_{mfp} = 3.67 cm
- 0.5*λ_{mfp} => minimum of 27 patches, but oct-tree on cube uses powers of 8 => 64 patches

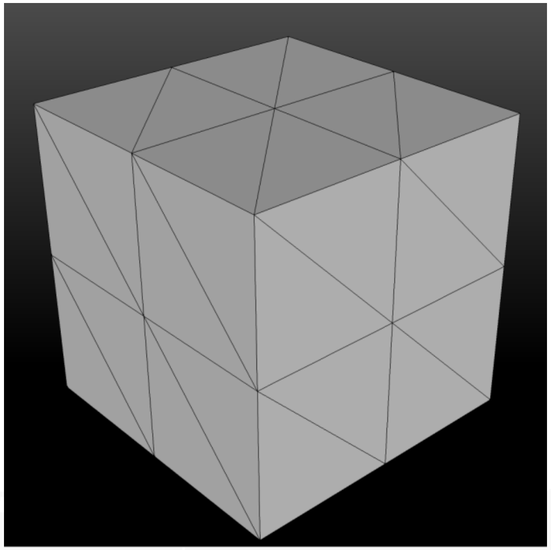
3 Meshes



fine mesh
56,557 elements
1,696,710 particles



patched mesh
64 patches
1,920 particles



coarse mesh
96 elements
2,880 particles

- **Adjust particle weighting → approximately 30 particles per element or patch**

Accuracy Comparison

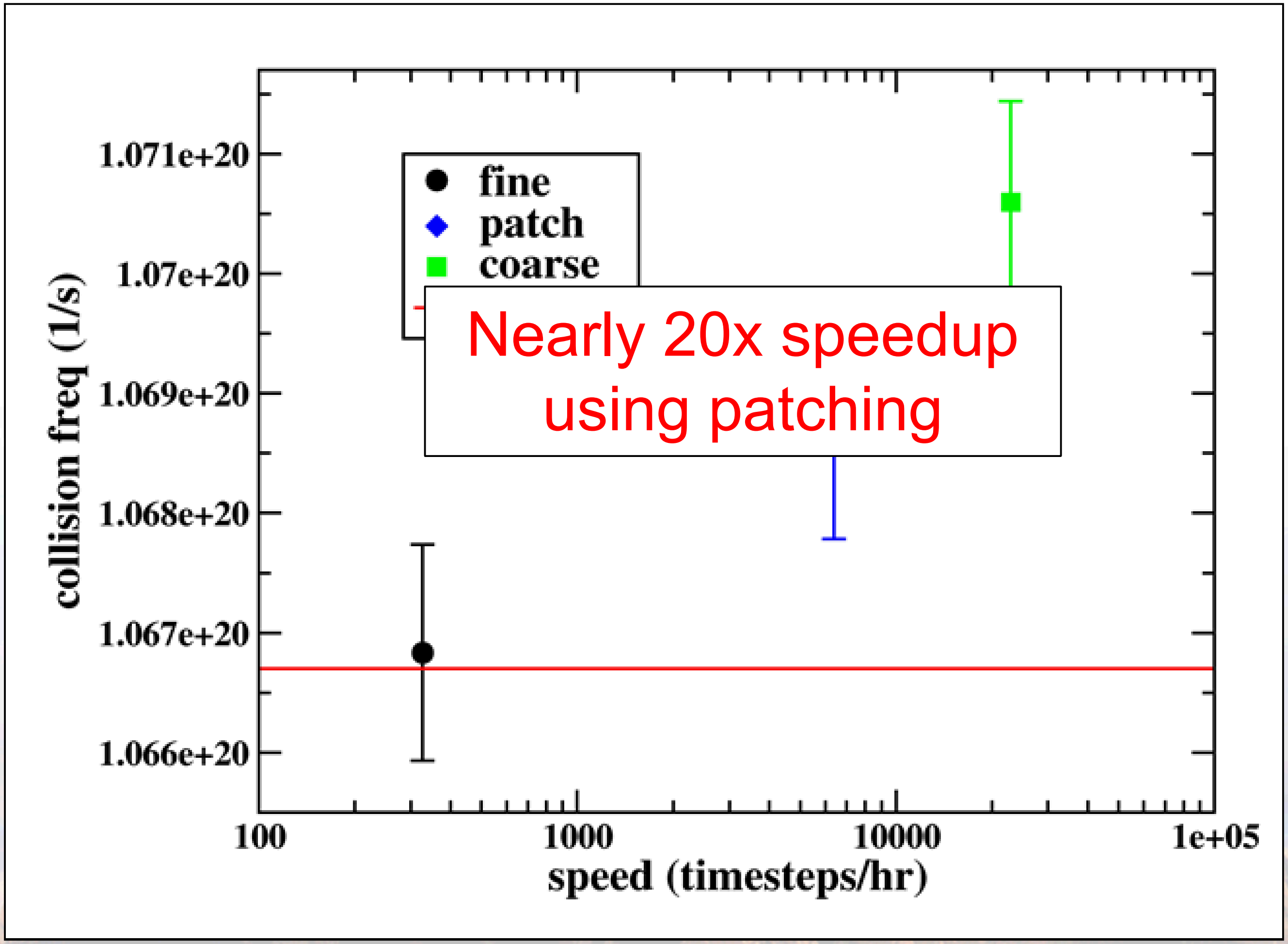
Ran each simulation for 3 hours ($\Delta t = 10^{-5}$ s) on one processor, repeated 6 times with a different random number seed

Average Collision Frequency:

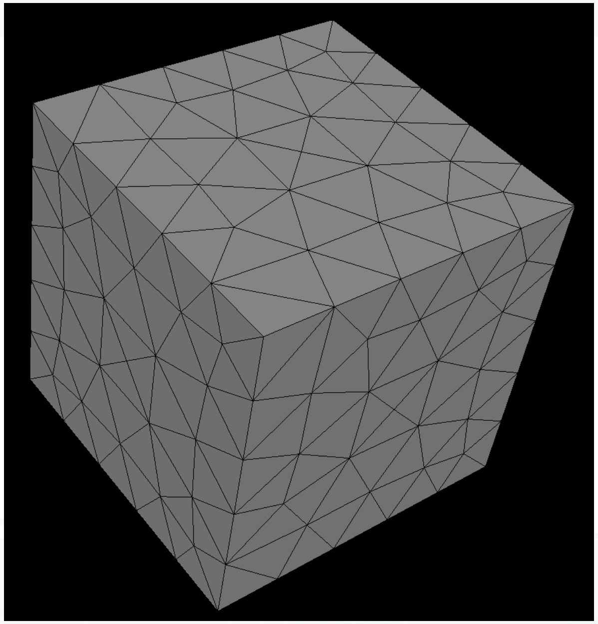
- $f_{analytic} = 1.0667 \cdot 10^{20}\ s^{-1}$
- $f_{fine} = 1.0668 \cdot 10^{20}\ s^{-1}$ → 0.01% relative error
- $f_{patch} = 1.0686 \cdot 10^{20}\ s^{-1}$ → 0.18% relative error
- $f_{coarse} = 1.0703 \cdot 10^{20}\ s^{-1}$ → 0.33% relative error

Results for the HI Test Problem

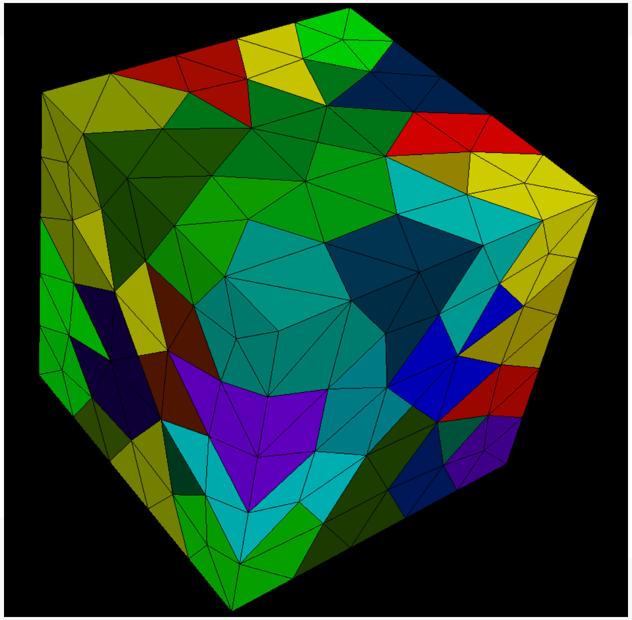
- Error bars represent 95% confidence intervals



Another 2 Meshes



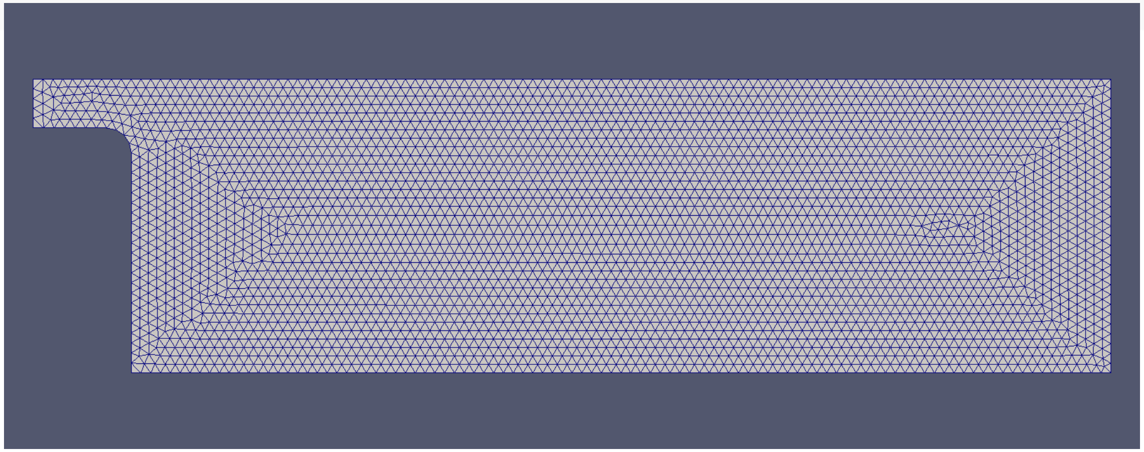
fine mesh
1,184 elements
1,223 particles



patched mesh
64 patches
1,223 particles

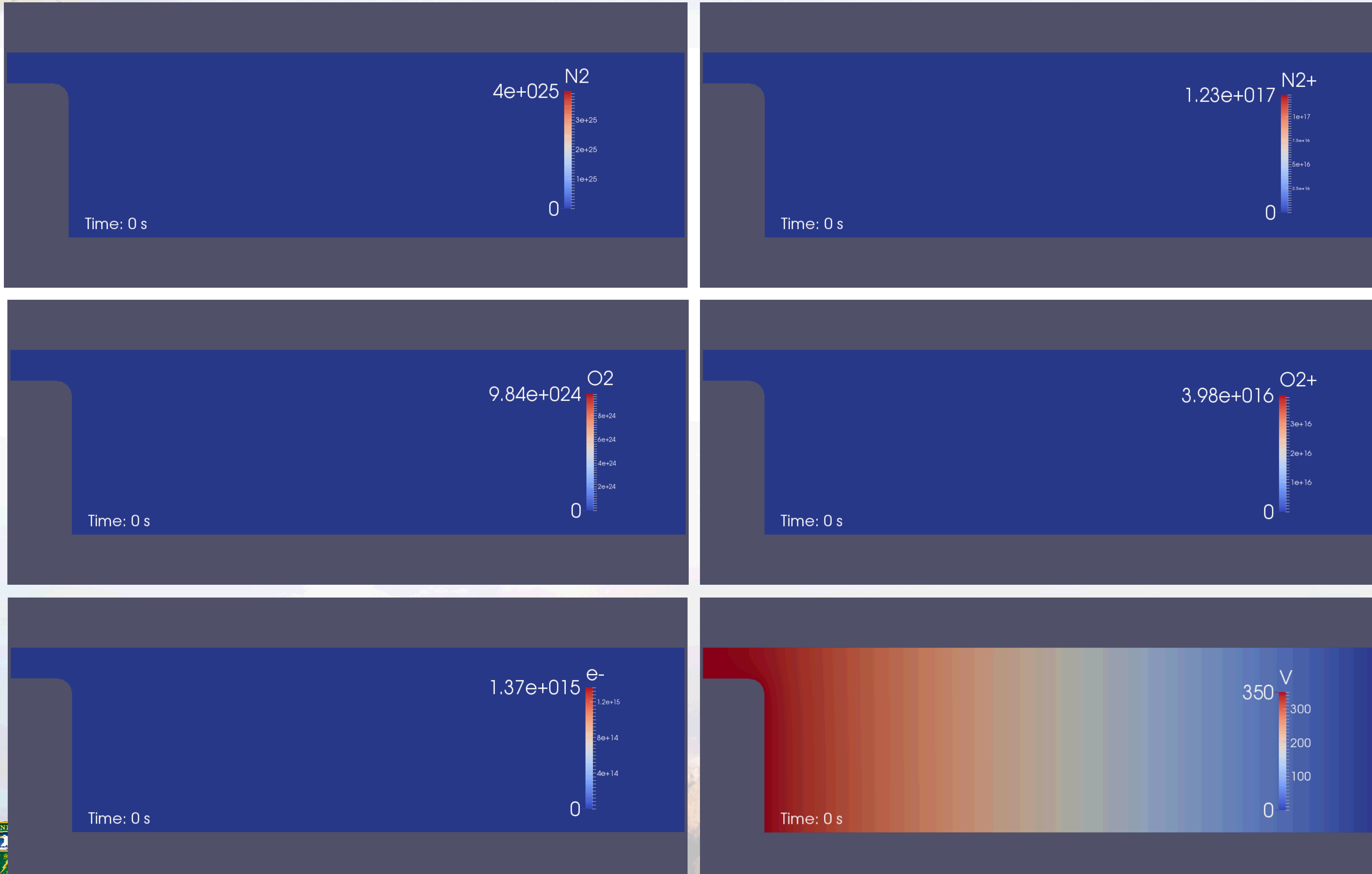
- **Same HI test problem (ran for 2000 timesteps)**
- **Patched mesh runs nearly 4x faster (with virtually the same accuracy)**

2D Vacuum Gap Breakdown



- **Air injected at high velocity and high temperature from the anode**
- **Low density electrons injected from the cathode**
- **Air ionizes and eventually will form plasma and break the gap**

Species Densities (m^{-3})



Dynamic Sizing of DSMC Collision Cells

Conclusions

- Developed a new method (patching) to enhance hybrid PIC-DSMC simulations
- Using fewer particles with patching gives similar accuracy and uncertainty as using a fine mesh with many particles
- Allows one to dramatically speed up the simulation if the PIC mesh is too small for DSMC collisions
- Allows one to dynamically adjust the size of DSMC collision cells on the fly (based on mean free path)

Thank You

Questions or comments?