

Introduction

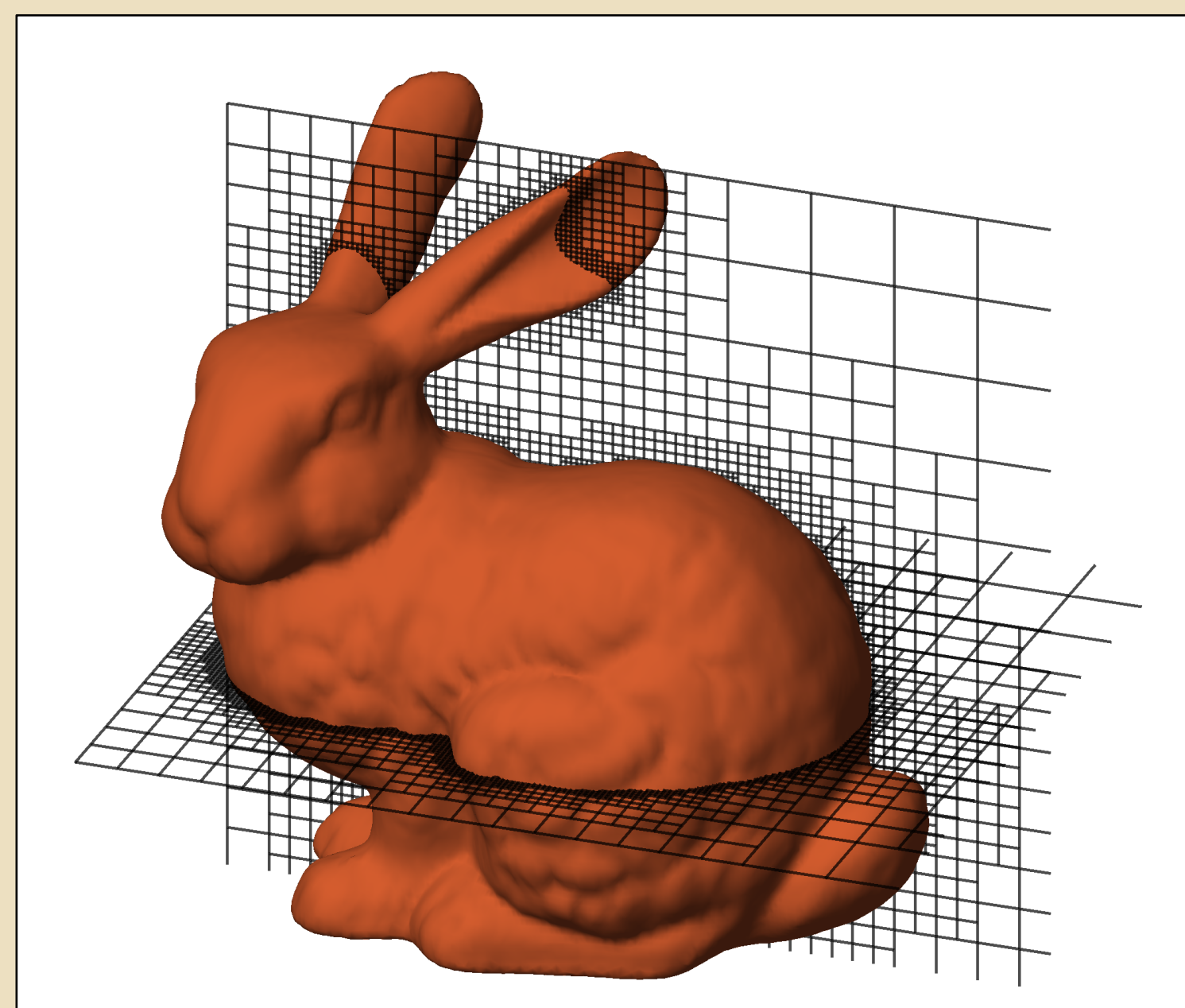
Many systems of interest in materials science can be described as two or more domains or phases separated by a thin interface. Modeling these systems is difficult because it often requires solving partial differential equations with boundary conditions on complicated or irregular boundaries. The smoothed-boundary method is a numerical technique that circumvents these problems by describing interfaces as diffuse regions where a phase-field-like parameter ψ varies smoothly between values defining separate domains. This powerful method allows us to solve PDEs within boundaries of arbitrary geometry; however, a high-resolution mesh is needed to accurately describe very thin interfacial regions—which on a uniform grid becomes computationally expensive. In order to increase the speed and accuracy of numerical simulations, we wish to apply adaptive mesh refinement to the smoothed-boundary method.

Project Goals

- Develop an algorithm to generate an adaptive Cartesian mesh from binary image or volume data
- Compare the efficiency and accuracy of the smoothed-boundary method on adaptive grids to sharp-interface solutions
- Demonstrate how our methods may be applied to problems in the area of fluid dynamics

Adaptive Mesh Refinement

Figure 1:
Our mesh generation algorithm applied to the Stanford Bunny test model



When solving PDEs using a finite-difference scheme, we describe our system as a connected grid of discrete nodes, or “mesh.” Adaptive meshing allows us to increase the density of grid points in regions that require greater detail and accuracy, such as the interface between two domains. In our algorithm, we take binary image or volume data, and apply level-set smoothing in order to obtain a diffuse interface. Next, our space undergoes quadtree (2D) or octree (3D) decomposition based on the gradient of the domain parameter, allowing us to have fine resolution in the region of the interface, and coarse in the bulk phases.

Numerical Methodology

Adaptive meshing allows us to effectively “shrink” the width of our diffuse interface by using a smaller grid spacing at domain boundaries, while still maintaining the same resolution of points across the interface. As the mesh becomes further refined, we see that our diffuse interface model approaches the sharp interface solution.

Accuracy Analysis

Figure 2: Comparison of Couette flow velocity profiles for uniform and adaptive grids at different levels of refinement

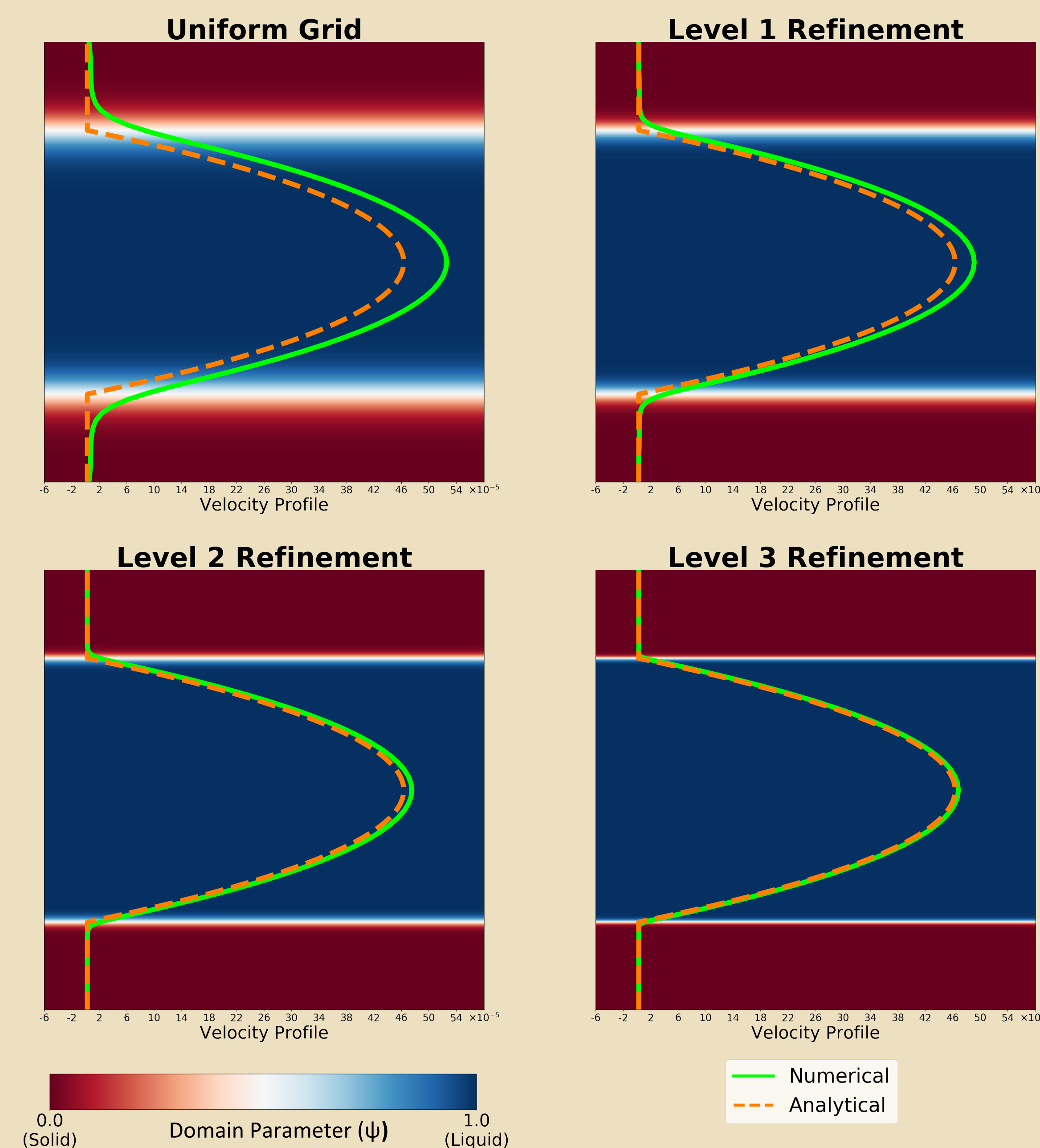
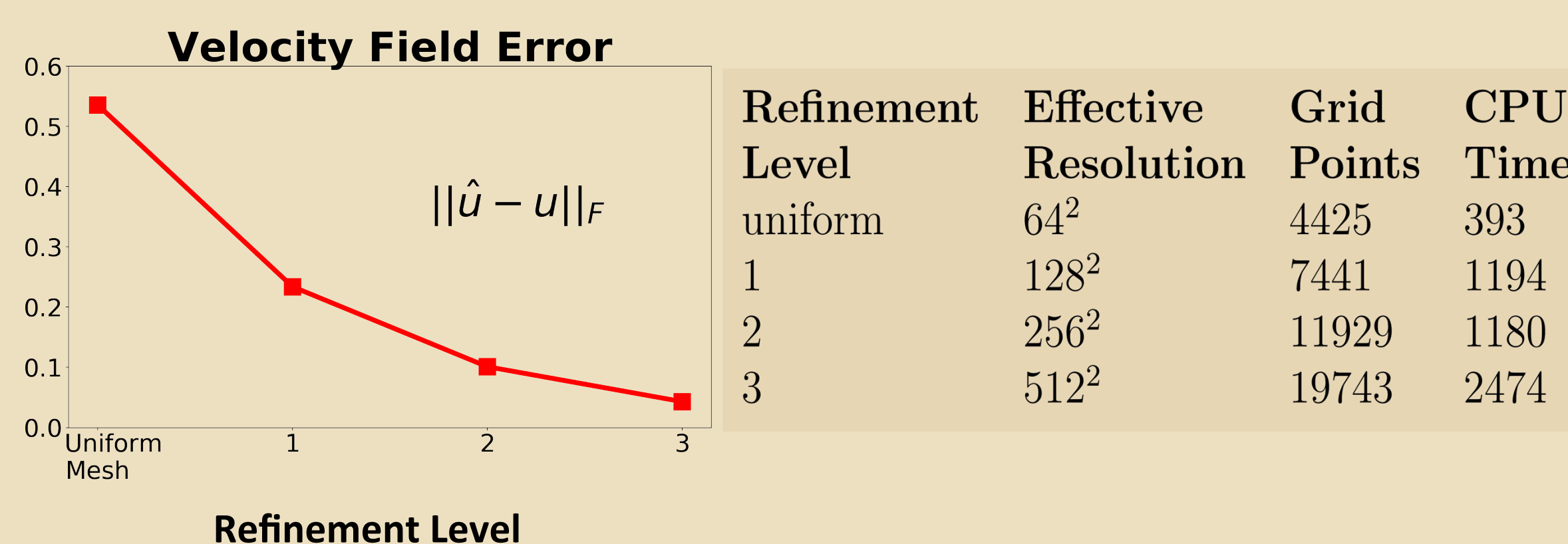


Figure 3: Error and Computational Resource Use for Fig. 2



Fluid Flow in Complex Geometries

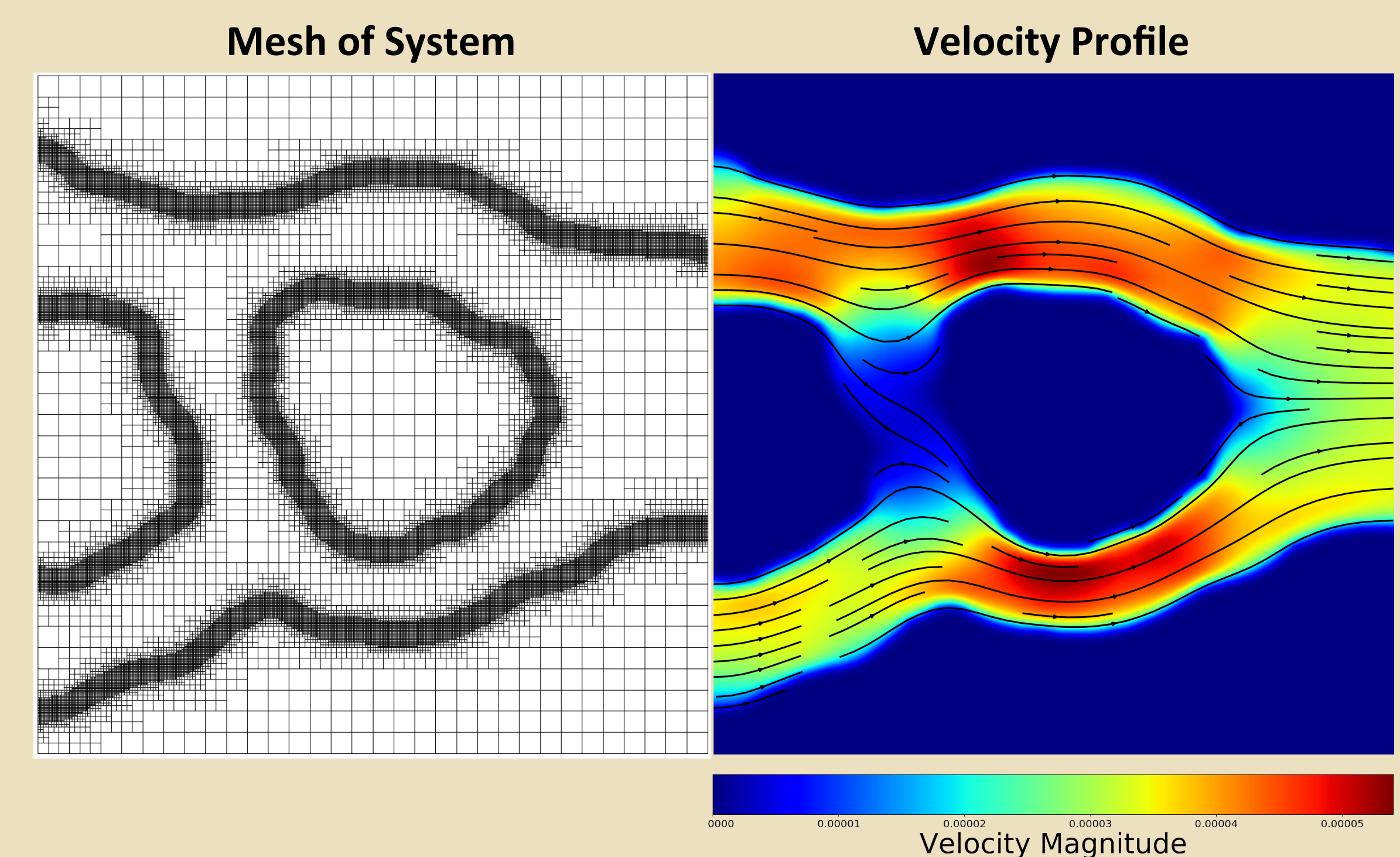
Equation 1: Navier-Stokes equations for incompressible flow

$$\frac{\partial \vec{u}}{\partial t} + (\vec{u} \cdot \nabla) \vec{u} = -\frac{1}{\rho} \nabla p + \nu \nabla^2 \vec{u} \quad \nabla \cdot \vec{u} = 0$$

Equation 2: Smoothed-Boundary formulation of Eq. 1

$$\frac{\partial \vec{u}}{\partial t} + (\vec{u} \cdot \nabla) \vec{u} = -\frac{1}{\rho} \nabla p + \underbrace{\frac{\nu}{\psi} (\nabla \cdot (\psi \nabla \vec{u})) - \frac{\nu}{\psi^2} (\nabla \psi \cdot \nabla (\psi \vec{u}) - B_D |\nabla \psi|^2)}_{\text{Boundary conditions imposed implicitly}}$$

Figure 4: Simulated flow through an irregular channel



Conclusions and Future Work

Adaptive mesh refinement has shown promise as a tool that can greatly increase the speed and accuracy of numerical simulations utilizing the smoothed-boundary method. Our experiments show that AMR allows us to selectively refine interfacial regions, yielding results that agree with sharp-interface and analytical solutions. Future work will involve applying our methods to more complex problems in materials science, such as two-phase flow through porous media.

Acknowledgments

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References:

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