Lattice Boltzmann Methods for Fluid Dynamics

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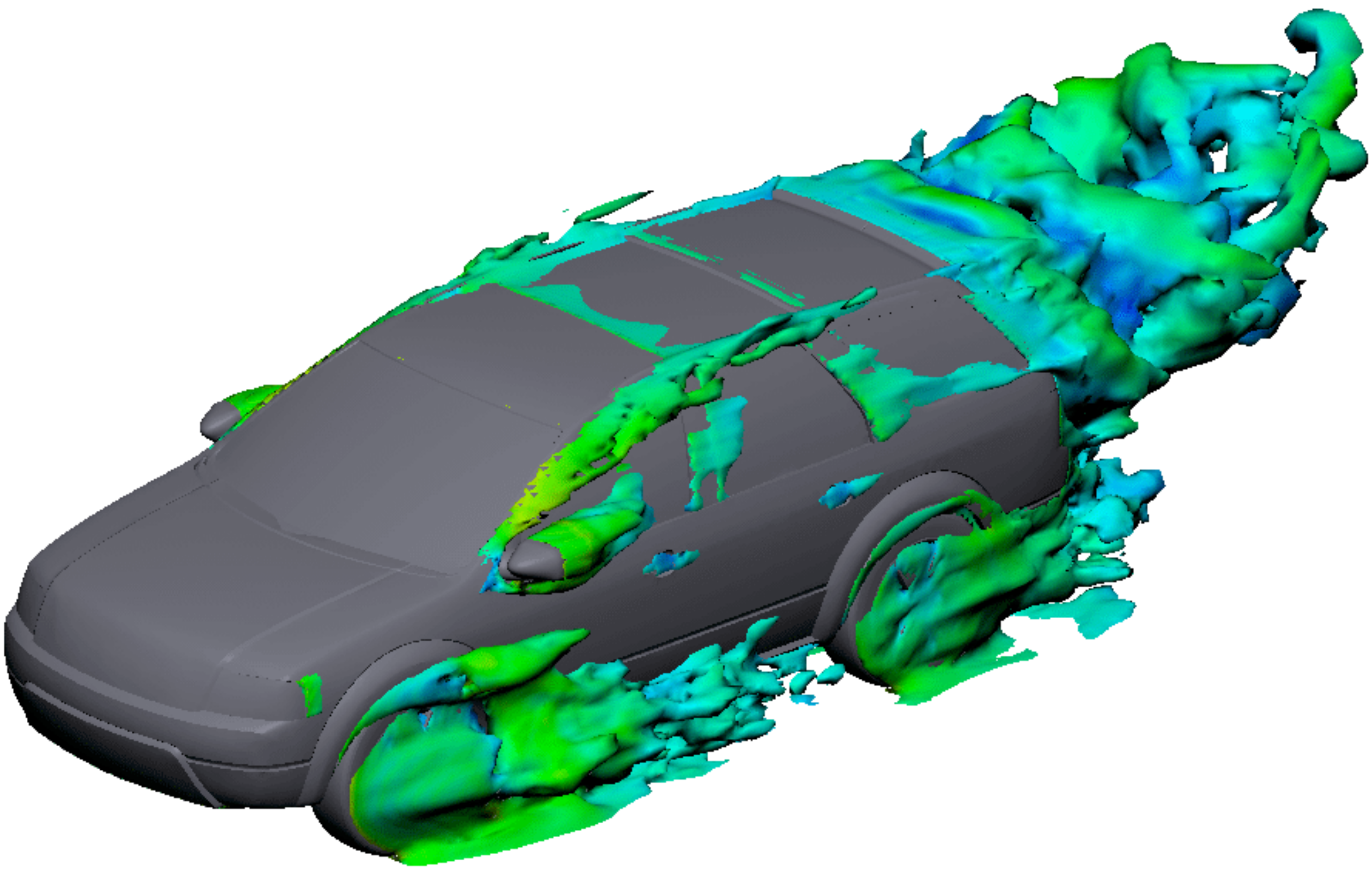
Transient flow around a car



LBGK vs. CONVENTIONAL CFD

Real Fluid
Free molecules in continous space

Continuum Kinetic Theory
Microscopic particles (Boltzmann Equation)

Conventional CFD Methods

Construction of fluid equations
Navier-Stokes equations (PDE)

Discrete approximation of PDE
Finite difference, finite element, etc

Numerical integration
Solve the equations on a given mesh and apply PDE boundary conditions

Lattice Based Method

Discrete formulation of kinetic theory
Lattice Boltzmann equations

No further approximation
The equations are already in discrete form

Numerical integration
Solve on lattices and apply kinetic based BC

Simple conversion to fluid variables
These are theoretically shown to obey the required fluid equations

Results
Fluid dynamic quantities at discrete points in space and time

Lattice Boltzmann (or BGK) Methods

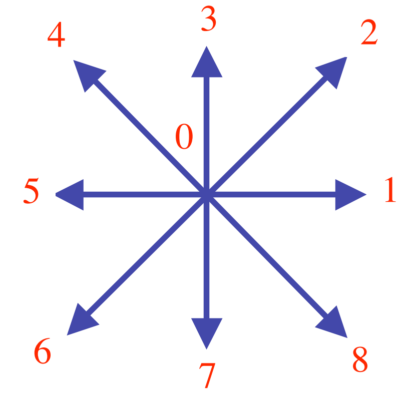
Particles only have a finite number of discrete velocity values

$$\vec{v} \to \{\vec{c}_i;\ i = 0, 1, \cdots, b\}$$

b in 3D ~ 20 - 30

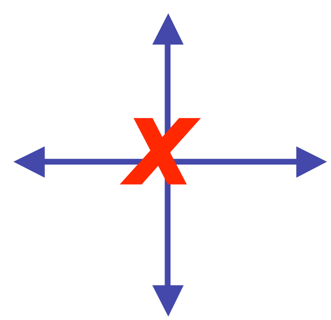
$$f(\vec{x}, \vec{v}, t) \to n_i(\vec{x}, t);\ i = 0, 1, \cdots, b$$

Number density for particles with velocity $\vec{c}_i$



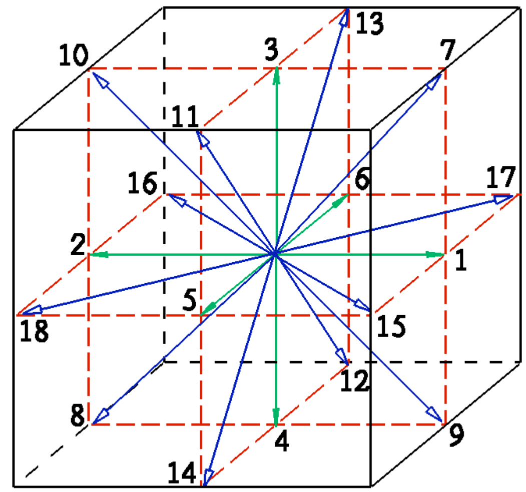
The choice is not arbitrary!

- *Satisfy foundational symmetry requirements (up to required orders)*
- *Avoid spurious invariants*



Lattice BGK method

LBGK:



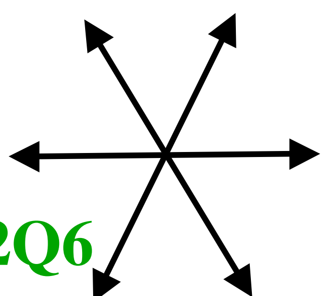
$$\boxed{n_i(\vec{x}+\vec{c}_i\Delta t, t+\Delta t) = n_i(\vec{x},t) + C_i(\vec{x},t)}$$

Coupled (via C_i) algebraic difference equations

BGK form: $$C_i = -\frac{1}{\tau}(n_i - n_i^{eq})$$

D3Q19 lattice

Fluid quantities obtained via averaging over $\vec{c}_i$ and space-time:

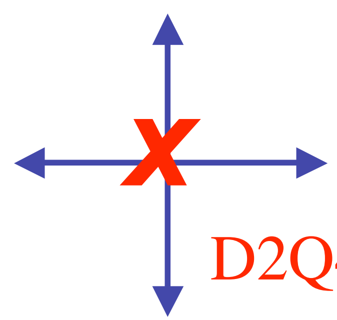


D2Q6 lattice

$$\rho = \sum_i n_i$$

$$\rho\,\vec{u} = \sum_i \vec{c}_i\, n_i$$

$$\rho\, T = \frac{1}{D}\sum_i (\vec{c}_i - \vec{u})^2\, n_i$$



D2Q4

Remarks on LBGK

- Lattice BGK yields the Navier-Stokes equations
    - Chapman-Enskog asymptotic expansion in powers of Knudsen number λ/L or $\tau/T << 1$
- Easy to compute time dependent flows
- Relaxation time τ defines viscosity
- No need to compute pressure explicitly
- Boundary conditions are fully realizable
- Stability is ensured
- Parallel performance with arbitrary geometry

Brief Comparison of LBGK and Conventional CFD

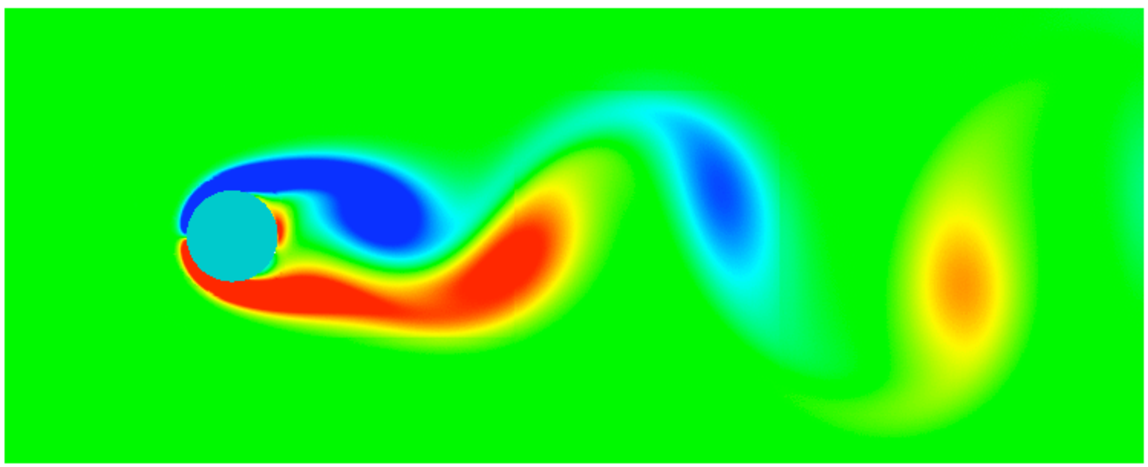
Conventional CFD

1. Nonlinear dynamic advection
2. Non-local – limited parallel performance
3. Issues with boundary conditions (BC)
4. Geometry setup slow
5. 3D time dependent flows costly to simulate
6. Complex physics (like multi-phase flows) require complex physical models

LBGK

1. Linear advection
2. Local and fully parallel
3. BC are fully realizable for arbitrary geometry
4. Geometry setup fast
5. Time dependent flows straightforward – especially important in 3D
6. Complex physics (like multi-phase flows) involve simple physical models

2D Cylinder



2D Cylinder

Re = 100

	Re =100	
	Cd	St
Exp.	…	0.164 (Williamson)
Braza et al.	1.364	0.16
Liu et al.	1.350	0.164
Calhoun	1.330	0.175
Henderson	1.35	0.167
PowerFLOW 4.0beta3	1.336	0.164

Braza et al. 1986, Finite volume with ADI (p-v NS), 2nd order accurate

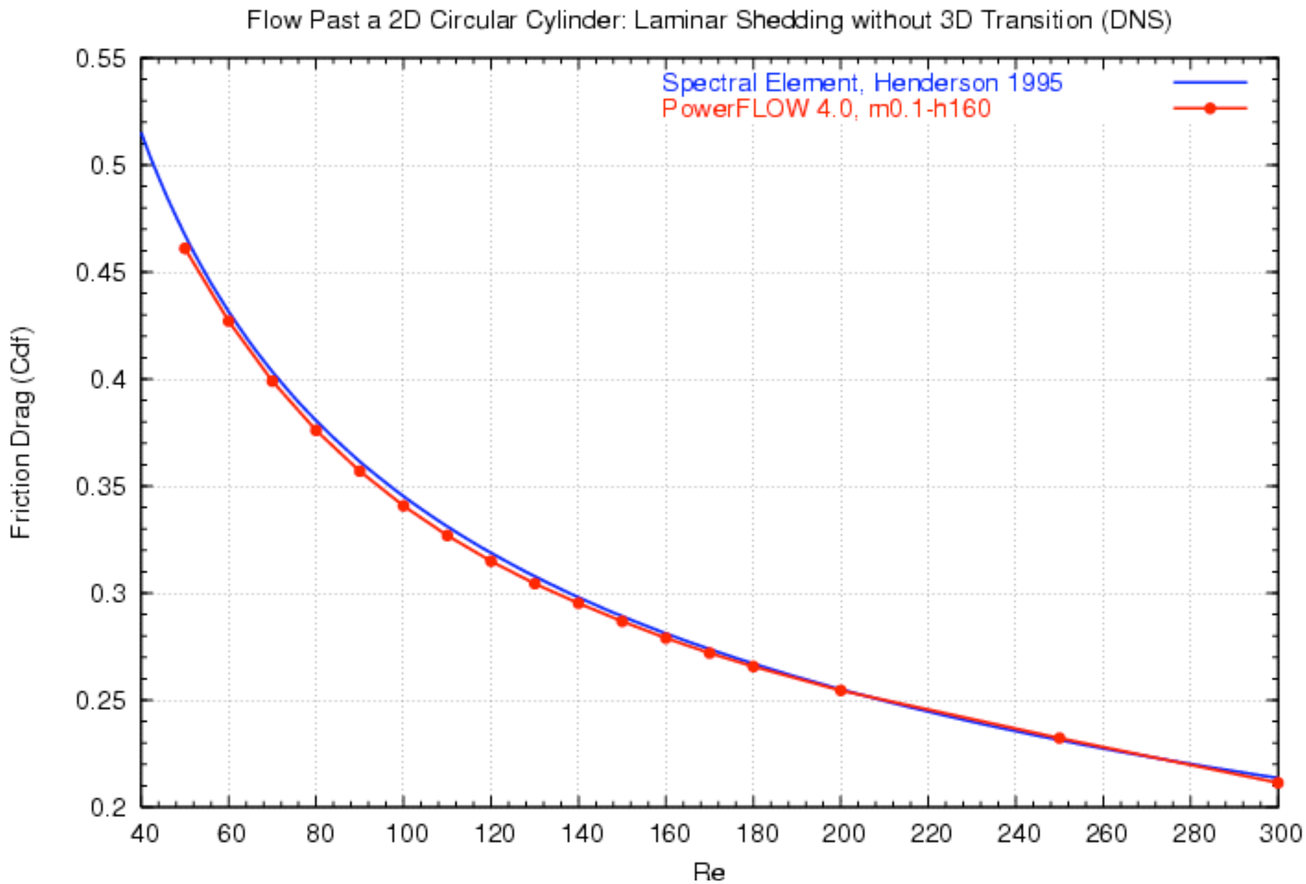
Liu et al. 1997, Finite volume with AC (p-v NS), preconditioned multigrid 2nd order central difference

Calhoun 2002, Cell centered Cartesian grid (s-v NS)

Henderson 1995, Spectral Element (NS)

2D Cylinder

Friction Drag



How do you derive N-S from LBGK?

- Chapman-Enskog (moment expansion) procedure in powers of Knudsen number λ/L
- Navier-Stokes equations are independent of orientation of coordinate system
- BUT – lattice BGK is highly anisotropic
- REMARKABLE FACT – isotropy of velocity moments only up to a fixed finite order are required

Isothermal Navier-Stokes equations at low Mach numbers

- Density/momentum

$$\rho(\mathbf{x},t) \equiv \sum_{\alpha=1}^{b} f_\alpha(\mathbf{x},t), \quad \rho\mathbf{u}(\mathbf{x},t) \equiv \sum_{\alpha=1}^{b} \mathbf{c}_\alpha f_\alpha(\mathbf{x},t)$$

- Momentum flux tensor

$$P_{ij}(\mathbf{x},t) \equiv \sum_{\alpha=1}^{b} c_{\alpha,i} c_{\alpha,j} f_\alpha(\mathbf{x},t)$$

- Energy flux tensor

$$Q_{ijk}(\mathbf{x},t) \equiv \sum_{\alpha=1}^{b} c_{\alpha,i} c_{\alpha,j} c_{\alpha,k} f_\alpha(\mathbf{x},t)$$

- **Navier-Stokes requires isotropy of velocity moments only up to 4th order**

High-order models

- Non-isothermal low Mach number Navier-Stokes equations requires velocity moment isotropy up to 6th order
- Other physically relevant models reuqire even higher-order velocity moment isotropy, further restricting the discrete velocity set used in lattice BGK
- For example, non-isothermal flow with Burnett corrections requires 8th order isotropy

Relation between rotational symmetry and order of moment isotropy in 2D

- *b* velocities $C = \{\mathbf{c}_\alpha = (cos(\frac{2\pi\alpha}{b}), sin(\frac{2\pi\alpha}{b}); \quad \alpha = 0,\ldots,b-1\}$ is invariant under rotations by multiples of $2\pi/b$
- Isotropy of the n^{th} order basis moment tensor

$$\mathbf{M}^{(n)} \equiv \sum_\alpha^b \mathbf{c}_\alpha \mathbf{c}_\alpha \ldots \mathbf{c}_\alpha$$

requires that $\sum_\alpha^b (\mathbf{c}_\alpha \cdot \hat{v})^n \stackrel{n}{=} A$ where A is a constant and $\hat{v} = (cos\,\theta, sin\,\theta)$ is any unit vector

- This requires that $h_b^{(n)}(\theta) \equiv \sum_{\alpha=0}^{b-1} cos^n(\frac{2\pi\alpha}{b} - \theta)$ be independent of θ, which holds if $\sum_{\alpha=0}^{b-1} e^{i\frac{2\pi\alpha}{b}(2j-n)} = 0$ ie (2j-n)/b is not a nonzero integer for j=0,…,n
- CONCLUSION: Isotropy for so $n \leq b-2$ hexagonal lattice gives 4th order isotropy, etc.

3D Moment Isotropy

- n^{th} order basis moment tensor

$$\mathbf{M}^{(n)} = \sum_{\alpha=1}^{b} w_\alpha \underbrace{\mathbf{c}_\alpha \otimes \mathbf{c}_\alpha \otimes \cdots \otimes \mathbf{c}_\alpha}_{n}$$

- Isotropy requires

$$M^{(n)}_{\underbrace{i \cdots i}_{n}} = \frac{(n-1)c^2}{D+n-2} M^{(n-2)}_{\underbrace{i \cdots i}_{n-2}}$$

$$M^{(n)}_{\underbrace{i \cdots i}_{n-2} jj} = \frac{(n-3)c^2}{D+n-2} M^{(n-2)}_{\underbrace{i \cdots i}_{n-4} jj}$$

$$M^{(n)}_{\underbrace{i \cdots i}_{n-4} jjjj} = \frac{(n-5)c^2}{D+n-2} M^{(n-2)}_{\underbrace{i \cdots i}_{n-6} jjjj}$$

and so on

Generation of N^{th} order isotropic lattices

- Using these relations an N^{th} order isotropic lattice can be constructed by a union of $(N\text{-}2)^{nd}$ order isotropic lattices and its rotated realizations
- Example: 6th order set with 59 velocities

1	(0,0,0)	12	$\{(\pm 1,\pm 1,0),(\pm 1,0,\pm 1),(0,\pm 1,\pm 1)\}$
6	$\{(\pm 1,0,0),(0,\pm 1,0),(0,0,\pm 1)\}$	8	$\{(\pm 1,\pm 1,\pm 1)\}$
6	$\{(\pm 2,0,0)\}$	12	$\{(\pm 2,\pm 2,0),(\pm 2,0,\pm 2),(0,\pm 2,\pm 2)\}$
8	$\{(\pm 2,\pm 2,\pm 2)\}$	6	$\{(\pm 4,0,0),(0,\pm 4,0),(0,0,\pm 4)\}$

Boltzmann-τ Turbulence Modeling

- Turbulence modeled *via* a modified relaxation time $\boldsymbol{\tau}$

$$\frac{\partial f}{\partial t} = -\frac{1}{\tau}(f - f^{eq})$$

$$\frac{1}{\tau} = \frac{1}{\tau_{turb}} + \frac{1}{\tau_{shear}} + \frac{1}{\tau_{buoyancy}} + \frac{1}{\tau_{swirl}} + \ldots$$

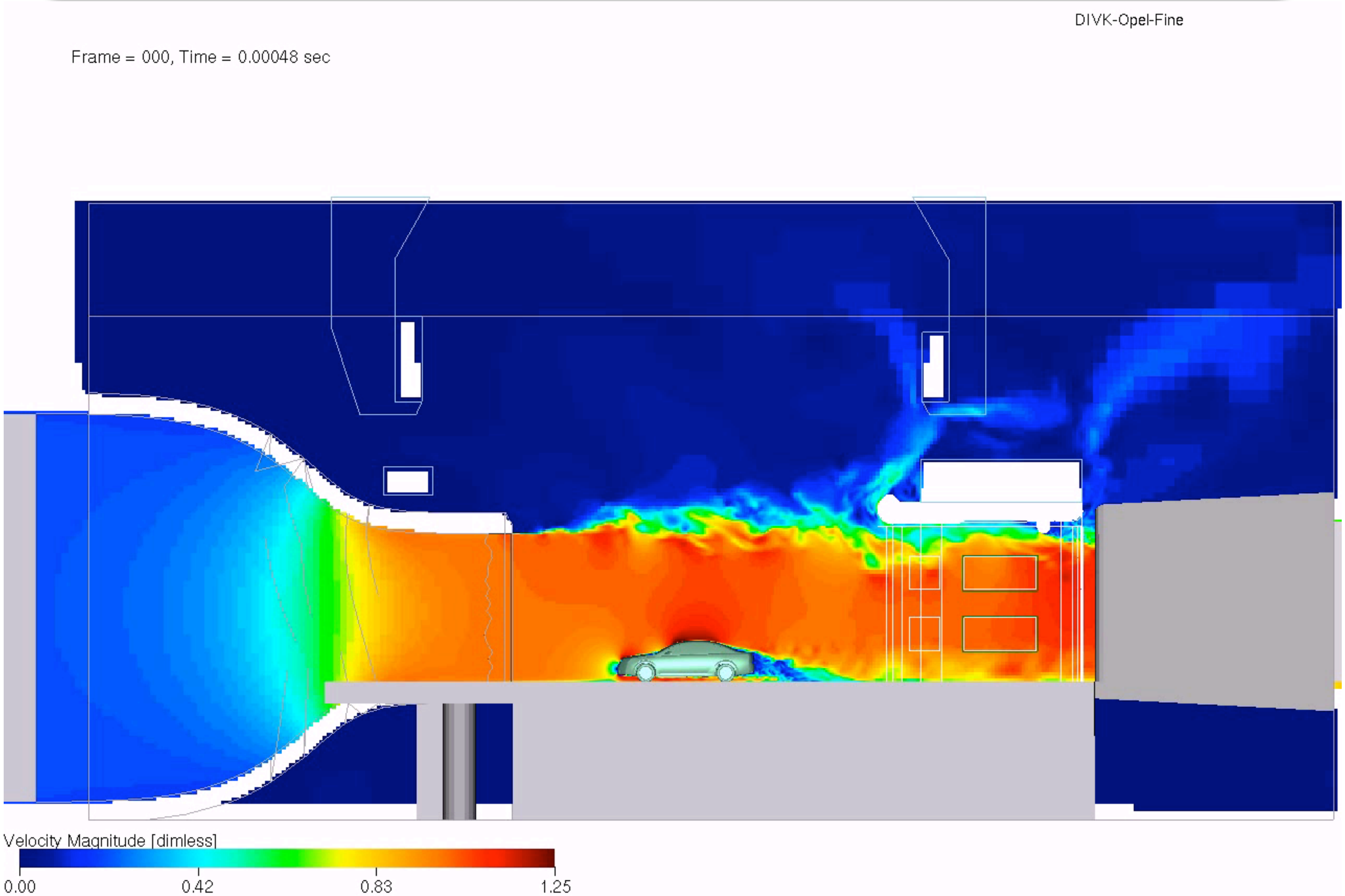
Advantages of Boltzmann-τ Method - I

- Realizability of the turbulence model
- Boltzmann-τ has guaranteed realizability
  - *Requires only* $\tau_{\mathrm{turb}} > 0$
  - *Stable numerical results*
  - *Positive eddy viscosity*
- Navier-Stokes-based turbulence models can have significant difficulties with realizability
  - *Divergent turbulence quantities*
  - *Negative eddy viscosities, …*

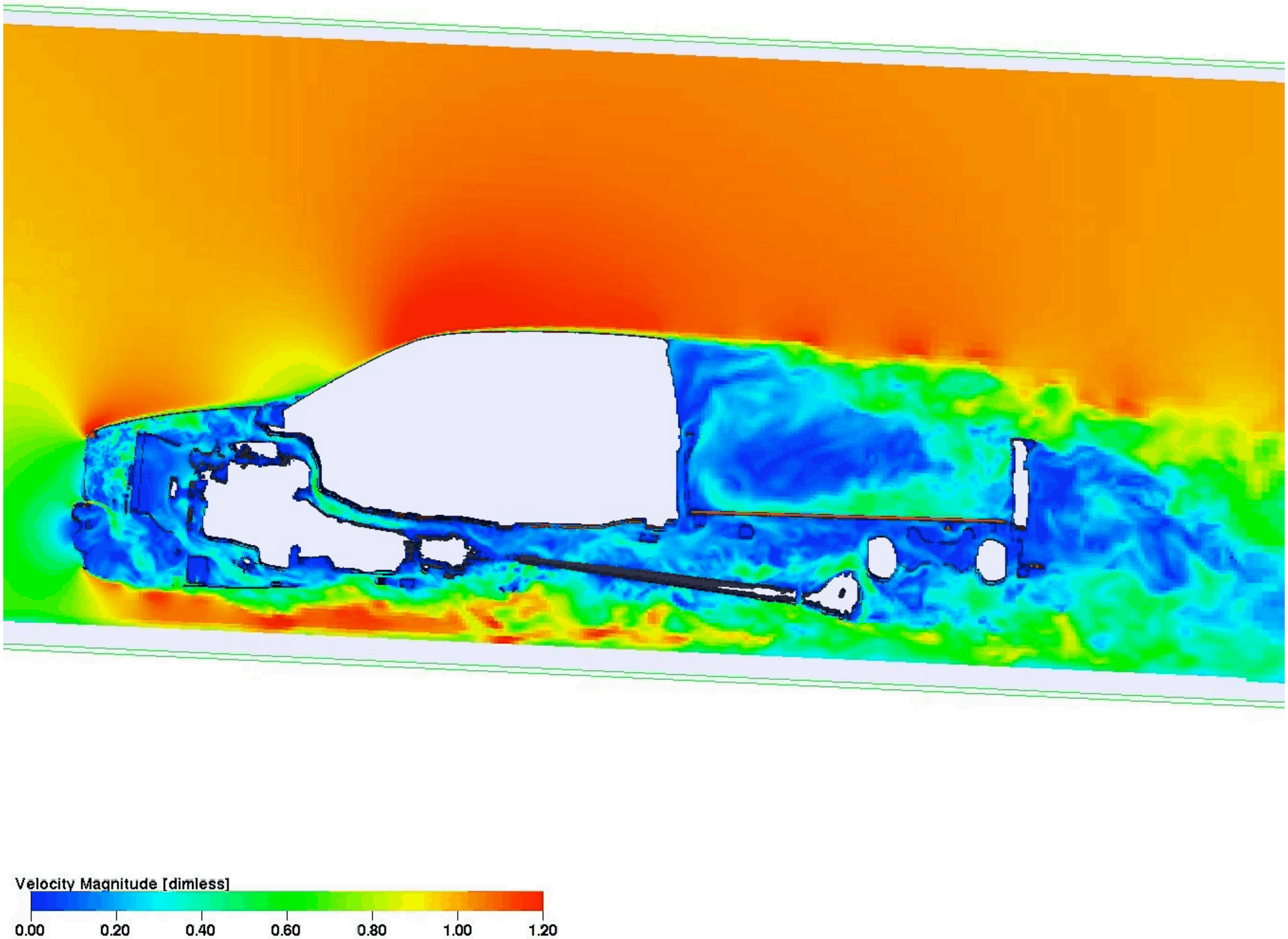
Advantages of Boltzmann-τ Method - II

- With the BGK model in terms of space, time, and velocity as independent coordinates, simple approximations (like τ models) may be extraordinarily complex in fluid (velocity/pressure) variables
- Fluid velocity/pressure are projections of the BGK variables onto a lower-dimensional space
- In contrast to higher-order Chapman-Enskog projections, the BCs on BGK are well defined and easy to implement

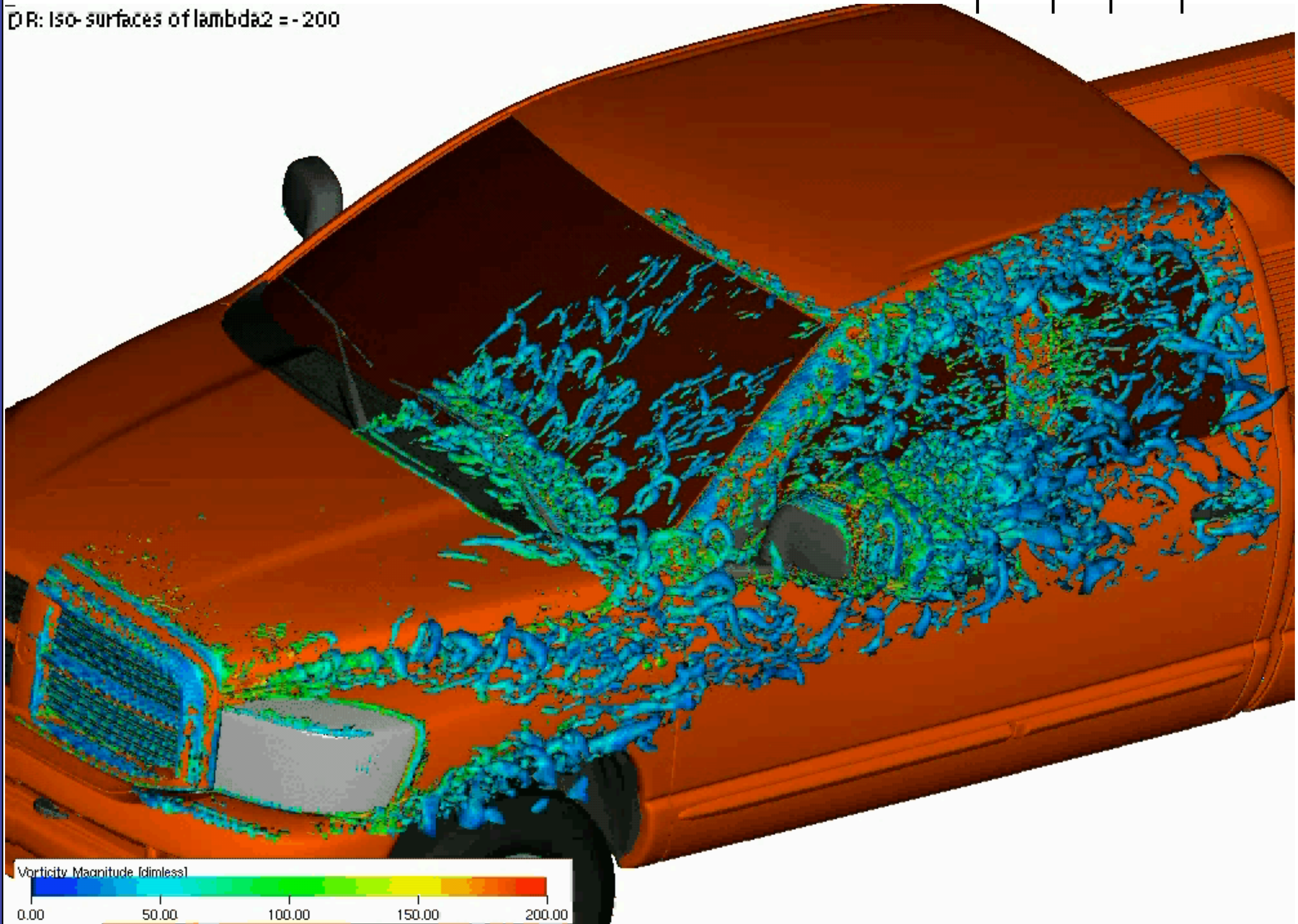
An Opel in a Wind Tunnel
Centerline Velocity at 140 km/h



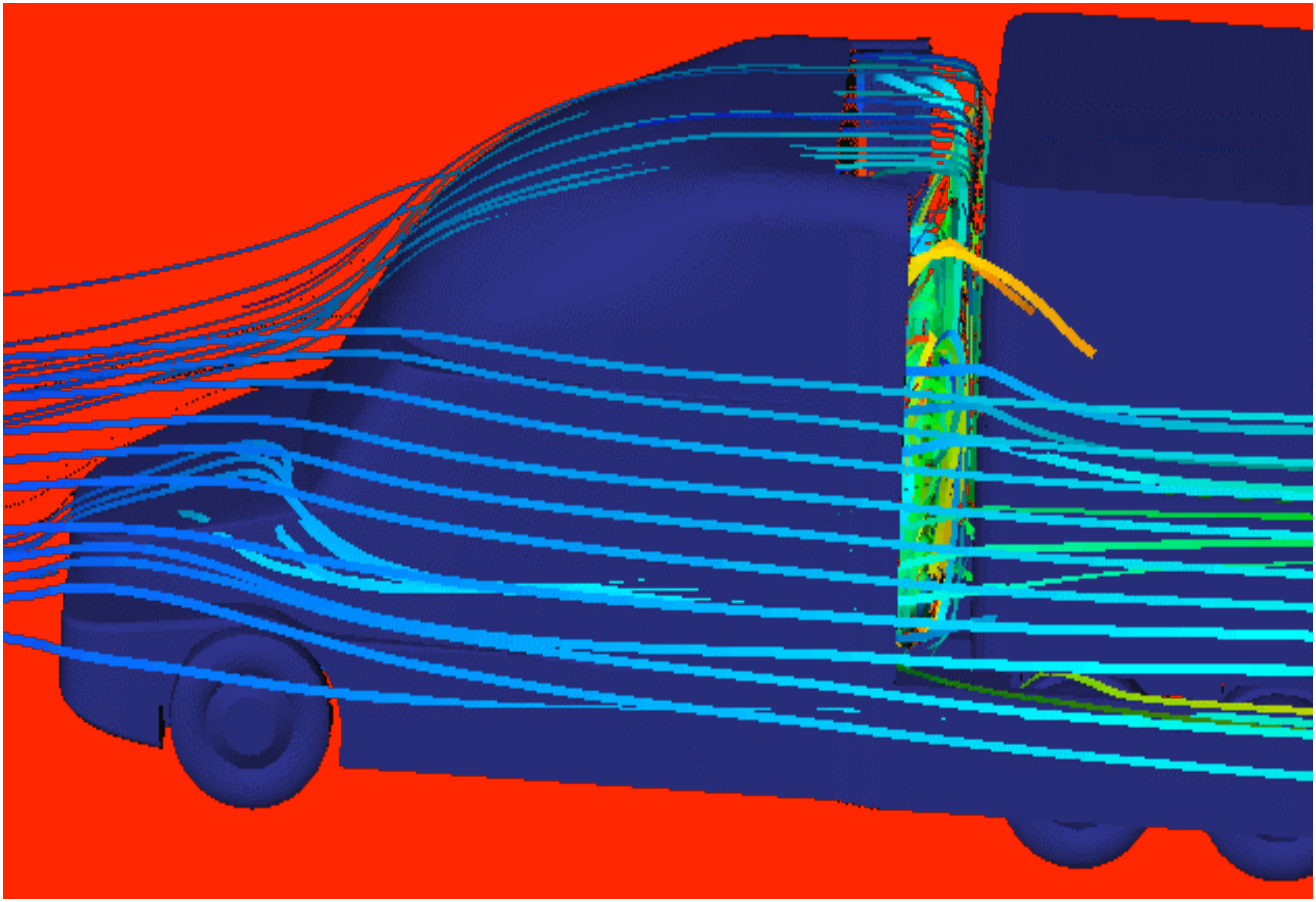
Dodge RAM – Exterior/underhood/ under-carriage flow – centerline velocity



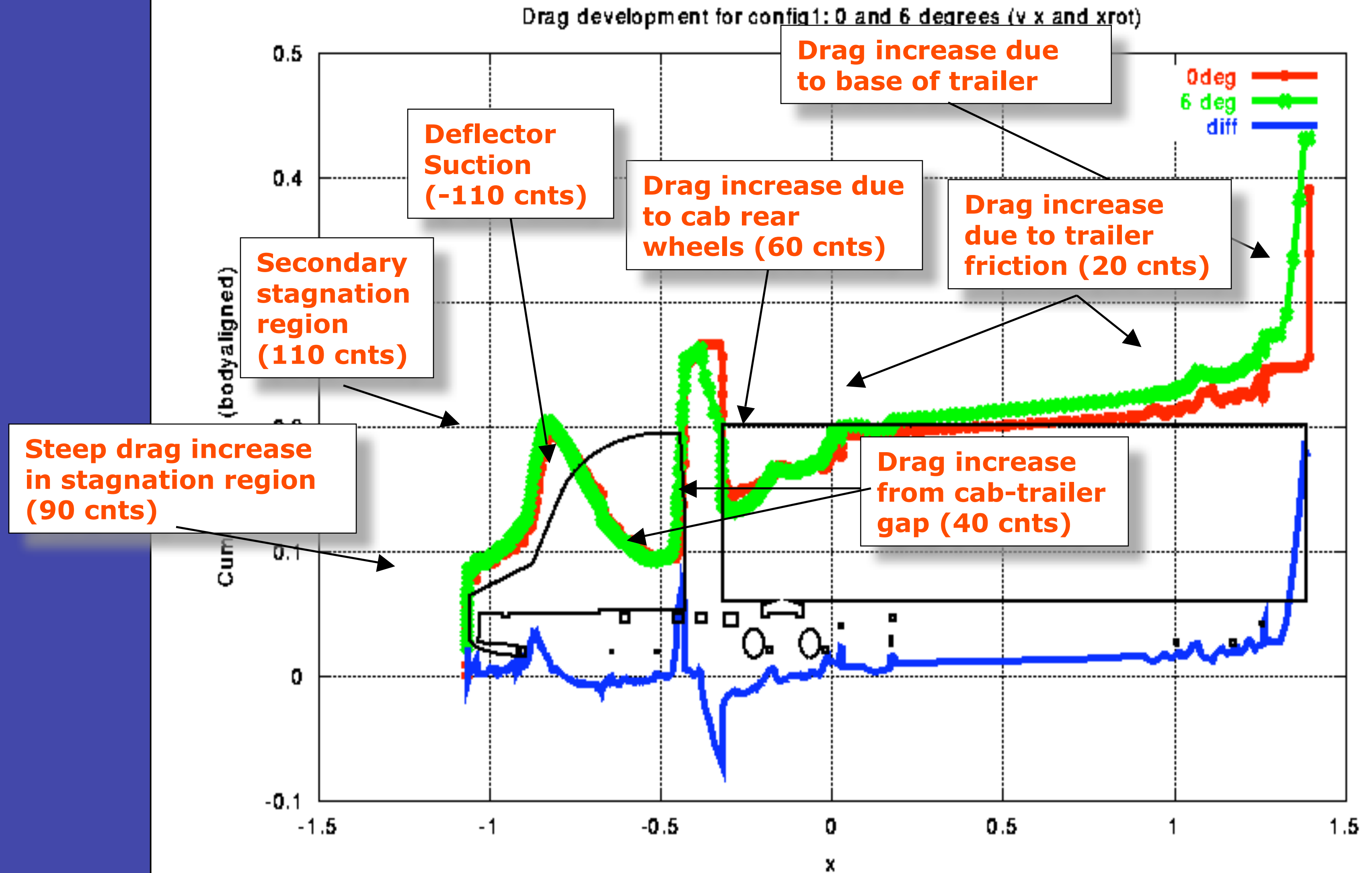
Dodge RAM – Acoustic Impact of Headlight/Hood Design on A-Pillar and Door Seals: $\lambda_2 = \left|\omega^2\right| - \left|S^2\right|$



3D Streamlines of Flow Past a Large Truck



Drag Development



Conclusions

- Lattice BGK allows straightforward mix of complex fluids, complex physics, and complex geometries
- Appropriate lattice structures can be derived to assure accurate and efficient flow computations, even with turbulence and other complex physics included