Scalable Adaptive Finite Element Framework for Multiphysics Simulations

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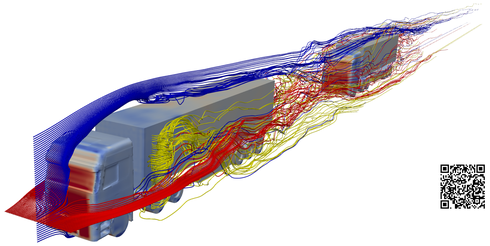
Motivation

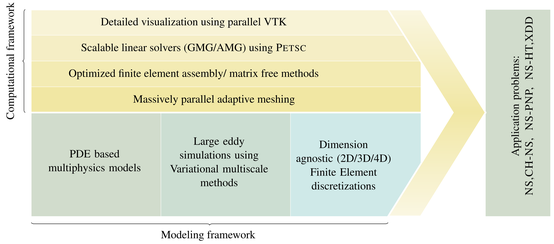
- **Solving multiphysics and multiscale problems.**
  - Adaptivity: an essential requirement to resolve accurate physics at multiple scales across space and time.
- **NASA 2030 Overnight LES challenge:**
  - 100,000 timesteps over 6 - 8 hours on a reasonably big mesh of 30–300 million elements.
  - Targeted towards optimization/design problem: Need remeshing each iteration.
  - *"Mesh generation and adaptivity continue to be significant bottlenecks in the CFD workflow".*



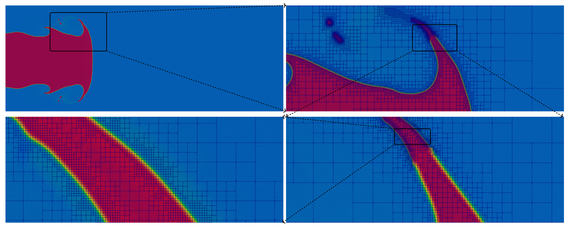
Streamlines of flow past two platooning trucks.

Contributions

- Massively parallel framework for efficient solution of PDEs over complex domains.
- Major challenges addressed:
  - Scalable adaptive mesh generation over complex domains – incomplete octrees (Technical Contribution 1).
  - Efficient data structures and algorithms to expose parallelism in modern clusters (Technical Contribution 2 – 4).
  - Scalable integration with numerical solvers (PETSc) (Technical Contribution 5).
  - Efficient and accurate numerical schemes (Application 1–4).
- All contributions released in an open–source code Dendrite-kt (https://bitbucket.org/baskargroup/dendrite-kt/src/master/)



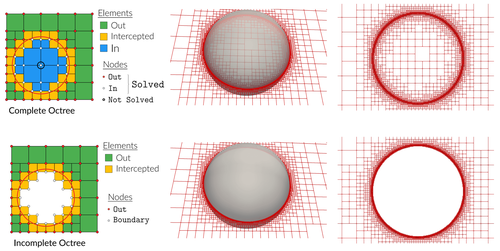
Importance of adaptivity in capturing multiscale phenomena.



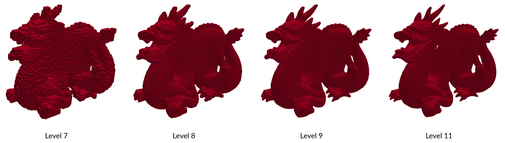
Element size vary by a factor of 1000 in each dimension

Technical contribution 1: Incomplete octree generation

- An *incomplete* octree framework – capable of carving out any complex object based on simple In - Out test.

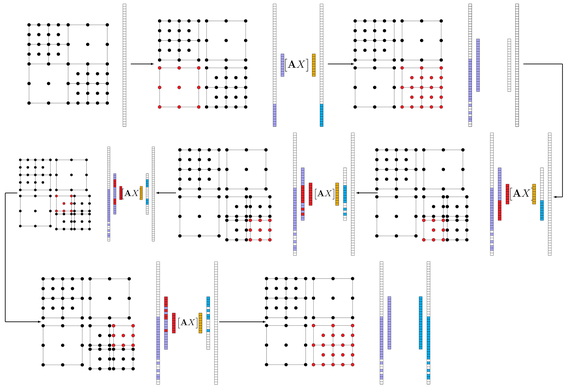


- Stanford Dragon:



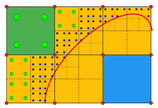
Technical contribution 2: Traversal based MatVec

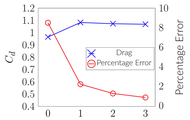
- Global to local nodal maps lead to indirect memory access - Not ideal to exploit deep memory hierarchy of modern super-computer.
- Our approach - Perform MatVec in a recursive top-down and bottom-up fashion.



Technical contribution 3: Adaptive quadrature

- Obtained by recursive subdivision of Intercepted cells.
  - Volume integration happens only for Out Gauss points.
- Essential for accurate volume integration.
- Do not add to any extra degrees of freedom.



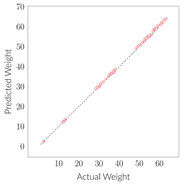


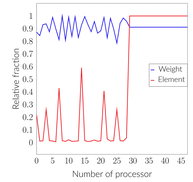
Technical contribution 4: Dynamic Load Balancing

- Theoretical estimate for load on each element:

$$W(e) = \frac{n_{\mathrm{Vgp}}(e)}{n_{\mathrm{Tgp}}} + \frac{T_s}{T_v}\frac{n_{\mathrm{Sgp}}(e)}{n_{\mathrm{Tgp}}}$$

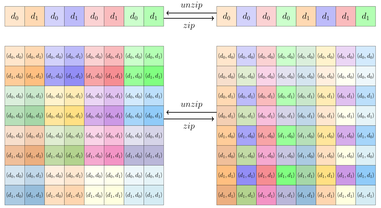
  - T_v volumetric quadrature evaluation cost
  - T_s surface point evaluation cost
  - n_{Vgp}: number of Out Gauss point
  - n_{Sgp}: number of surface Gauss points per element
  - n_{Tgp}: total number of volumetric Gauss points
- Weighted SFC partitioning to ensure load balance computation.



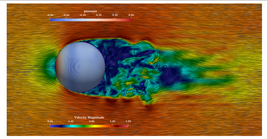


Technical contribution 5: Acceleration of matrix and vector assembly

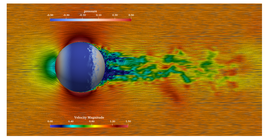
- PETSc block data storage: ideal for multi–dof system
- However, such storage: not ideal for local assembly.
  - Any FEM operator $(\mathcal{L}(u), \mathcal{L}(v))$ leads to strided memory access.
- Perform unzip operation followed by zip operation for best of both world.
- Further, express FEM operator as matrix - matrix multiplication / matrix - vector multiplication for matrix and vector assembly.



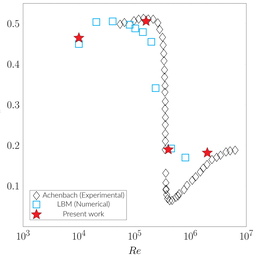
Application 1: Modeling turbulent flow – Capturing drag crisis



$\mathbf{Re} = \mathbf{10,000}$

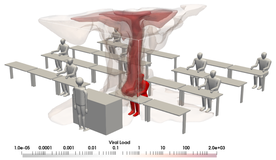


$\mathbf{Re} = \mathbf{2 \times 10^6}$

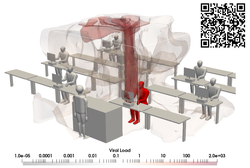


Drag variation with Re

Application 2: Modeling turbulent flow with heat transfer



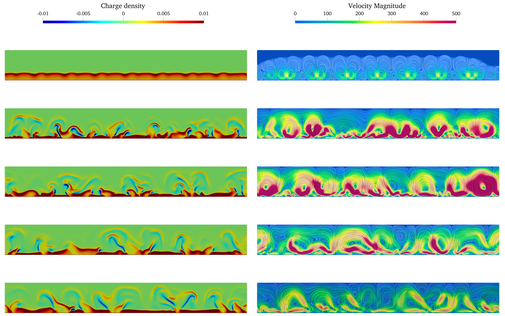
Without monitors



With monitors

Covid risk assessment in classroom – isocontours of viral load with red mannequin infected with Covid.

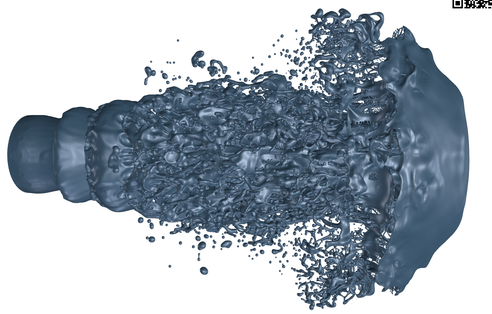
Application 3: Complex electrochemical modeling – Navier–Stokes + Poisson Nernst Planck



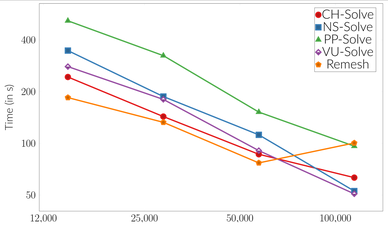
Electro-convective instability

Application 4: Primary Jet atomization – Cahn-Hiilard Navier–Stokes

- Most detailed simulation of jet atomization.
- Equivalent to 35 trillion grid points on the uniform grid - $64\times$ more resolved than the previous best.



Scaling on TACC Frontera



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- Saurabh, Kumar, et al. "Industrial scale Large Eddy Simulations with adaptive octree meshes using immersogeometric analysis." CAMWA 97 (2021): 28-44.
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