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High-order AMR computations of chemically reacting flows

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Motivation

Why AMR and High-Order Discretization ?

- Use AMR with a low Mach projection scheme to tackle the length-scale challenge of chemically reacting flows
- High-order (4) spatial discretizations allow same accuracy with fewer grid points as low-order
  - fewer chemical source term evaluations
  - shallower grid hierarchies; simpler load balancing

Outline

- Computational Methodology
  - Low-Mach number equations
  - Numerical construction
  - Adaptive mesh refinement
- Numerical Results
  - Flame-vortex interaction
  - Convergence rates & computational efficiency
- Summary and future work

Low-Mach Number Model

Transport equations:

$$\nabla \cdot \mathbf{v} = -\frac{1}{\rho}\frac{D\rho}{Dt}$$

$$\frac{\partial \mathbf{v}}{\partial t} = -\frac{1}{\rho}\nabla p + C_U + D_U$$

$$\frac{\partial T}{\partial t} = C_T + D_T + S_T$$

$$\frac{\partial Y_k}{\partial t} = C_{Y_k} + D_{Y_k} + S_{Y_k} \qquad k = 1 \rightarrow N_s$$

1. Momentum transport - pressure projection
2. Operator-split stiff approach
3. Momentum transport - pressure projection

Equation of state:

$$P_0 = \frac{\rho \Re T}{\bar{W}} = \rho \Re T \sum_{k=1}^{N_s} \frac{Y_k}{W_k} = \text{const}$$

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Momentum advance:

Adams-Bashforth: $\mathbf{v}^n \xrightarrow{C_U + D_U} \hat{\mathbf{v}}^{n+1}$

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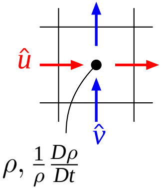

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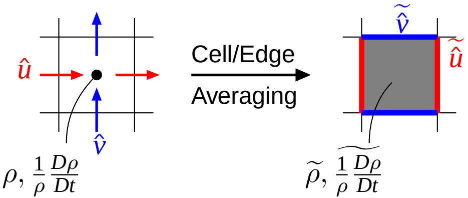

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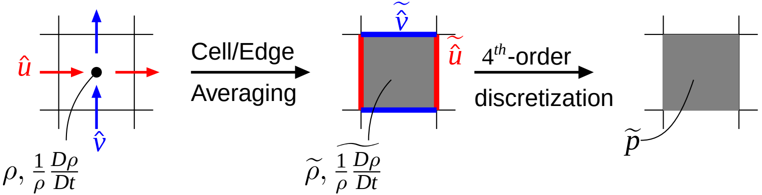

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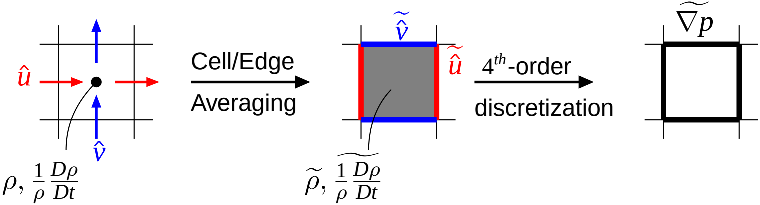

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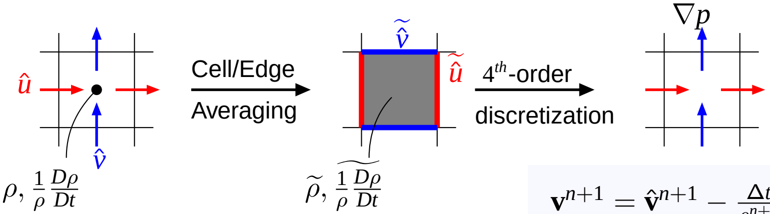

$$\mathbf{v}^{n+1} = \hat{\mathbf{v}}^{n+1} - \frac{\Delta t}{\rho^{n+1}} \nabla p$$

Scalar Advance

Symmetric Strang splitting: $\frac{R}{2}(C + D)\frac{R}{2}$

$$\Phi^{*} - \Phi^{n} = \int_{\Delta t/2} S_{\Phi} dt \qquad (CVODE)$$

$$\Phi^{**} - \Phi^{*} = \int_{\Delta t} (C_{\Phi} + D_{\Phi})\, dt \qquad (RKC2)$$

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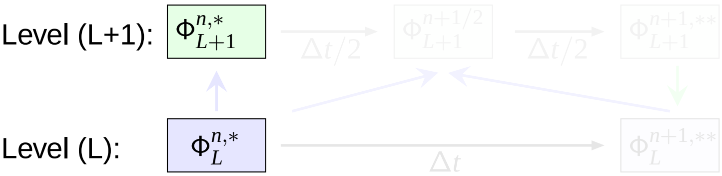

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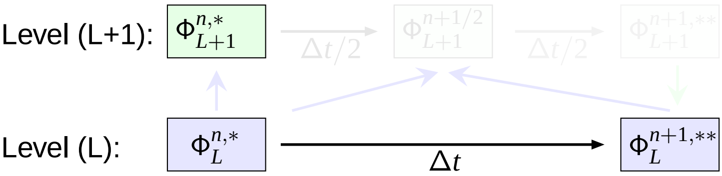

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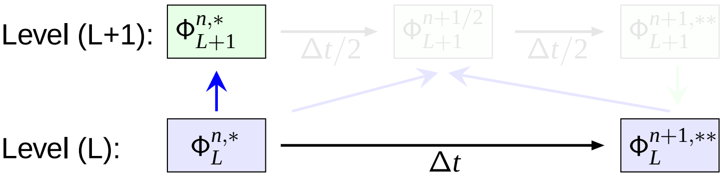

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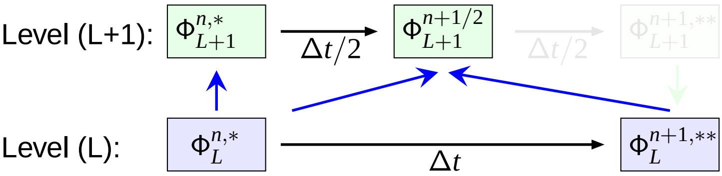

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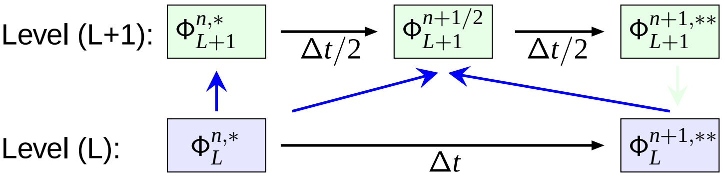

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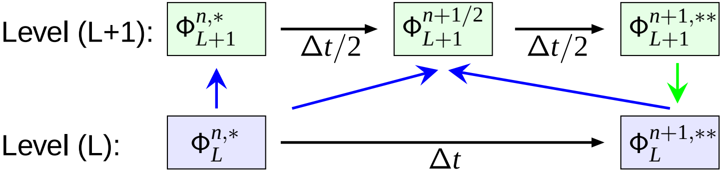

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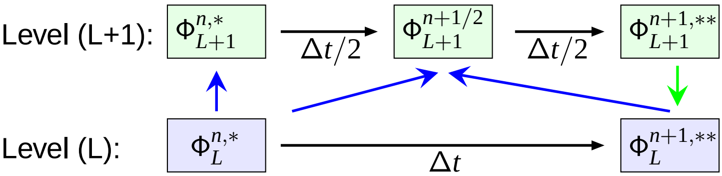
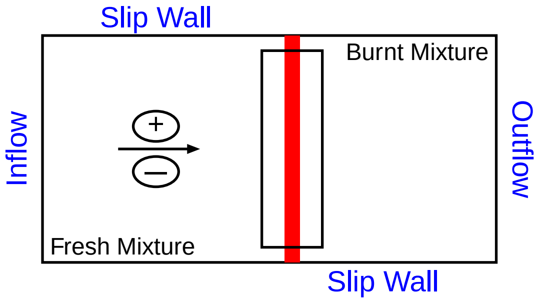


Numerical Construction - Summary

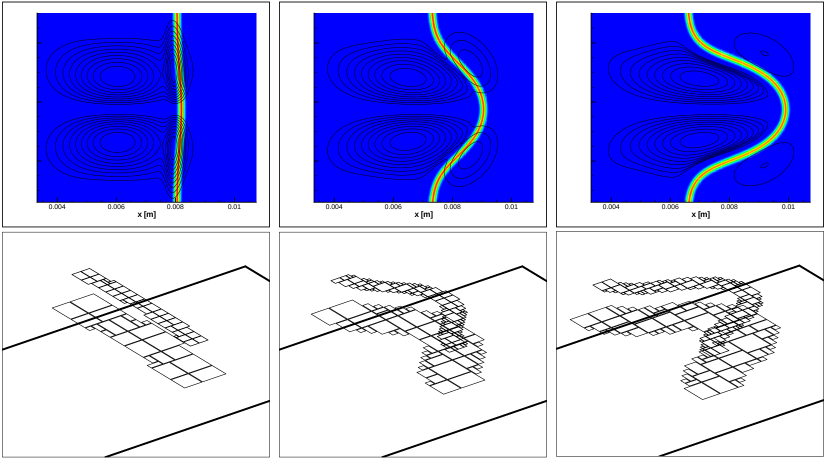
- The numerical construction uses a **hybrid approach**: momentum solved on a uniform mesh coupled with scalar transport in an AMR framework.
  - Spatial stencils: derivatives (4^{th} order), interpolations (6^{th} order), filters (8^{th} order); Time stencils: 2^{nd} order
- **Projection scheme**
  - Time integration: Adams-Bashforth
  - Variable coefficient Poisson equation: multigrid pre-conditioned CG solver (Hypre package)
- **Scalar update**: operator-split stiff approach with Berger-Colella time refinement
  - Convection/Diffusion advanced using Runge-Kutta-Chebyshev
  - Reaction advanced using BDF2 (cvode)
- **Chombo** library is used to handle the AMR infrastructure.

Flame-Vortex Dynamics



- IC: counter-rotating Lamb-Oseen vortices superimposed over a freely-propagating premixed flame (stoichiometric CH_4-air).
- GRI-Mech v3.0 (53 species, 325 reactions).
- 3 mesh levels: coarse grid size $60\mu m$

Flame-Vortex Dynamics



0.02ms 0.27ms 0.52ms

Convergence Rates

- Measured using:
  - succesivelly refined coarse grids and time step sizes
  - 1D (freely propagating premixed flame) and 2D (flame-vortex pair) configurations
- Time Convergence: $1.5625 \times 10^{-8} \rightarrow 5 \times 10^{-7}$s
  - Velocity field: **2.0**, Pressure: **1.8-2.0**, Scalars: **1.8-2.0**
- Spatial Convergence: $3.75 \rightarrow 30\mu$m (on the coarse level) and 2-3 refinement levels
  - Velocity field: **3.8-3.9**, Pressure: **3.6-3.9**, Scalars **3.6-4.0**

(Safta, Ray, Najm, JCP 2010, vol. 229)

Computational Expense of Algorithm Components

Stages

1. Momentum Projection
   - Velocity Predictor/Corrector
   - Pressure Solve
2. Scalar Advance
   - Reaction
   - Convection + Diffusion
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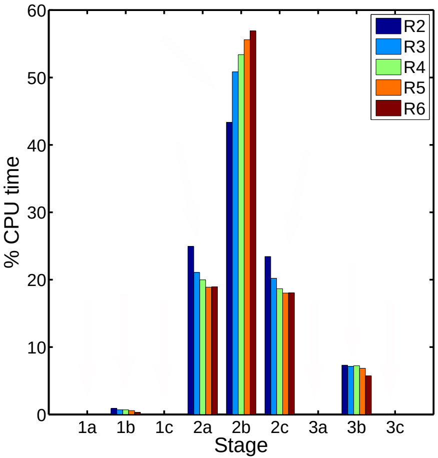

- C1 chemistry and mixture averaged transport properties
- R2 - uniform level run (512×256)
- R3-R6 - 2 level runs; fine level covers 5-30% of the coarse level

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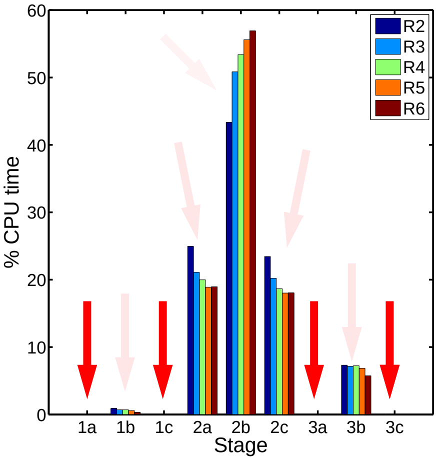

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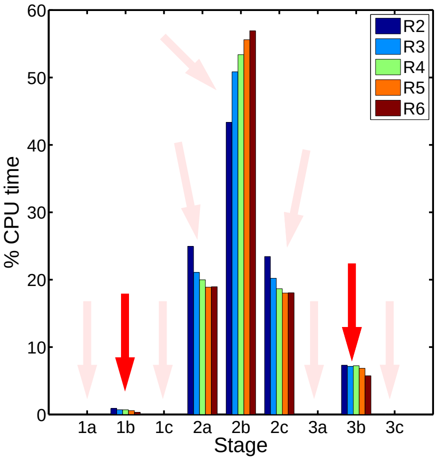

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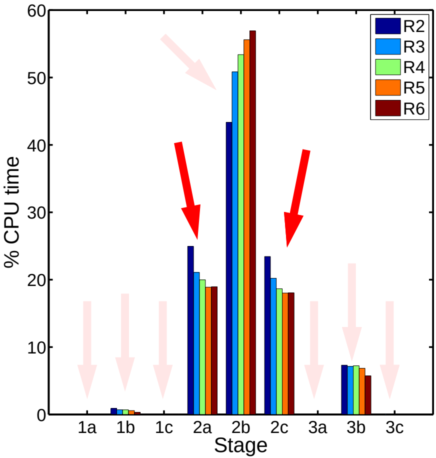

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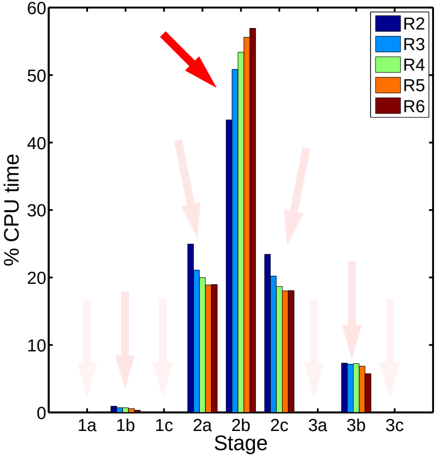

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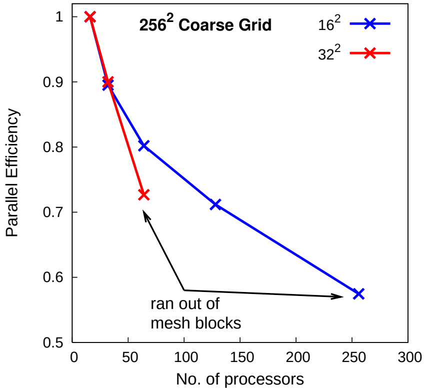
Computational Efficiency

- Preliminary results with small computational meshes. Tests with larger mesh sizes are ongoing.

AMR vs Uniform Mesh (UM)

1. 2 Level Mesh
   - Fine Level covers **5-30**% of the Coarse Level
   - CPU AMR/UM = **17-37**%
2. 3 Level Mesh
   - Finest Level covers **5-7**% of the Coarse Level
   - CPU AMR/UM = **8-12**%



- GRI-Mech 3.0 and mixture averaged transport properties

Summary and Future Work

- We have presented a high-order AMR construction for low Mach number reacting flow
  - Using a hybrid approach: pressure projection scheme on a uniform mesh coupled with a operator-split scalar transport on a AMR hierarchy
  - 2^{nd} order time convergence and 4^{th}-order spatial accuracy

Future work

- Continue working on improving the computational efficiency
- Study 2D laminar jet flames in laboratory-scale geometry with complex fuels.
- Couple this numerical construction with CSP-based time integration, adaptively reducing chemical stiffness and potentially eliminating operator-splitting.