Scalable Parallel Implementation of Numerical Simulation of Reacting Jet

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Combustion

Turbulence (Chaotic Property Changes – Occurs over a large range of length scales – *Integral to Kolmogorov*)

Reaction (Occurs over large range of time scales)

Computational Methods

RANS (Reynolds Averaged Navier Stokes - Modeling)
Time Averaged equations of motion
(Computationally Inexpensive but not very accurate)

LES (Large Eddy Simulation – Modeling)
Resolves large scales of flow and smaller scales are modeled
(Middle Ground)

DNS (Direct Numerical Simulation – No Modeling)
All Spatial and Temporal Scales are resolved
(Accurate but Computationally Very Expensive)

Accuracy of LES, RANS depends upon accuracy of models (mixing models – IEM, MC)

Validation of mixing models done by calculating relevant flow statistics (Scalar Dissipation Rate, Conditional Diffusion) [3]

Simulation of Spatially Evolving Mixing Layer to calculate Flow Statistics

1) Physical Boundary Conditions (Inflow / Outflow) against Periodic Boundaries used in Temporal Simulations
2) Accurate One Sided Finite Difference Stencil for computation on the boundaries (with least numerical diffusion)

MATHEMATICAL FORMULATION (at 1 atm pressure, constant properties , one-step reaction)

Continuity
$$\frac{\partial \rho}{\partial t}+\frac{\partial}{\partial x_j}[\rho u_j]=0;\ j=1,2,3$$

Navier Stokes
$$\frac{\partial}{\partial t}(\rho u_i)+\frac{\partial}{\partial x_j}[\rho u_i u_j+P\delta_{ij}-\tau_{ij}]=0,$$

Energy
$$\frac{\partial}{\partial t}(\rho e_t)+\frac{\partial}{\partial x_j}\left[(\rho e_t+P)u_j-Q_j+\sum_{\alpha=1}\bar{h}_{,\gamma}\bar{J}_{j,\gamma}-u_i\tau_{ij}\right]=-\dot{\omega}_p\Delta H^\circ;\ e_t=e+\frac{u_i u_i}{2}$$

Equation of State (Ideal Gas)
$$P=\rho\sum_x\frac{R^\circ}{W_x}T,$$

Transport Equation for Reacting Species
$$\frac{\partial}{\partial t}(\rho Y_\gamma)+\frac{\partial}{\partial x_j}[\rho Y_\gamma u_j-J_{j,\gamma}]=\dot{\omega}_\gamma;\ \gamma=O,F,P$$

Model for Heat Flux
$$Q_i=-\lambda\frac{\partial T}{\partial x_i},$$

Model for Mass Flux
$$J_{j,\gamma}=\rho\Gamma\frac{\partial Y_\gamma}{\partial x_j},$$

Source Term for Species
$$\dot{\omega}_O=-r\rho K_R(T)\left(\frac{W_P}{W_F}\right)Y_OY_F;\ \dot{\omega}_F=-\rho K_R(T)\left(\frac{W_P}{W_O}\right)Y_OY_F;\ \dot{\omega}_P=(1+r)\rho K_R(T)\left(\frac{W_P}{W_F}\right)\left(\frac{W_P}{W_O}\right)Y_OY_F$$

Reaction Coefficient
$$K_R(T)=A^0\exp\left[-\frac{E^0}{(R^0T)}\right]$$

Boundary Conditions

- 2D Simulations (Navier Stokes Characteristic Boundary Conditions – NSCBC: Euler Inviscid BC + Viscous Conditions) [2]
  - Inlet at x=0 – Subsonic Inflow
    - $U1, U2, T, Y_\alpha$ specified, Density Calculated from Continuity
    - Low Frequency Sinusoidal Perturbation Imposed (even without perturbation, Kelvin-Helmholtz type instability is seen in the Jet)
    - Viscous conditions: $\frac{\partial \tau_{xx}}{\partial x}=0, \frac{\partial q_1}{\partial x}=0$
  - Outlet at x=Lx – Non-reflecting outflow, Outflow Coefficient = 0.05, P_∞ imposed
  - Viscous conditions: $\frac{\partial \tau_{xy}}{\partial x}=0, \frac{\partial q_1}{\partial x}=0, \frac{\partial M_\alpha}{\partial x}=0$
  - Outlet at y=-Ly and y=Ly – Non-reflecting outflow, Outflow Coefficient = 0.4, P_∞ imposed
  - Viscous Conditions: $\frac{\partial \tau_{xx}}{\partial y}=0, \frac{\partial q_2}{\partial y}=0, \frac{\partial M_\alpha}{\partial y}=0$
- Case 1: Periodic Boundaries in z, Case 2: 3D NSCBC (for faces, edges and corners) [4]

Initial Conditions

$$\boldsymbol{w1}=[1-\tanh\left(\frac{\sqrt{\pi}\,x2}{D_{jet}}\right)\ \tanh\left(\frac{\sqrt{\pi}\,x2}{D_{jet}}\right)]$$
$$\boldsymbol{w2}=\tanh\left(\frac{\sqrt{\pi}\,x2}{D_{jet}}\right)$$

- Velocity Profile [U1= 86.8 m/s, U2=17.4 m/s]
$$U2+w1\,(U1-U2)$$
- Temperature Profile [T1=T2=300 K]
$$T2+w1\,(T1-T2)+2\left(\frac{(1+w)}{2}\right)\left(T_{flame}-\frac{1}{2}(T1+T2)\right);\ for\ y<0$$
$$+2\left(1-\frac{(1+w)}{2}\right)\left(T_{flame}-\frac{1}{2}(T1+T2)\right);\ for\ y>0$$
- Mass Fraction [mirrored across centerline]
$$Y2+w2\,(Y1-Y2)$$
- Fuel: Hexane, Oxidizer: Air
- Pr = Sc = 1, Ma= 0.25, Re = 800
- Da = 10, Ce = 3, Flame Temperature = 600 K

Numerical Approach

1. Temporal Terms - **Fourth Order Explicit Runge-Kutta** Time Integration
2. Spatial Terms –

Case 1 (stream wise (x_1) and cross stream (x_2))
- **Explicit Eighth Order Accurate Central Finite Difference scheme**
- **Boundary stencil - 3-3-4-6-8 Scheme** [1]

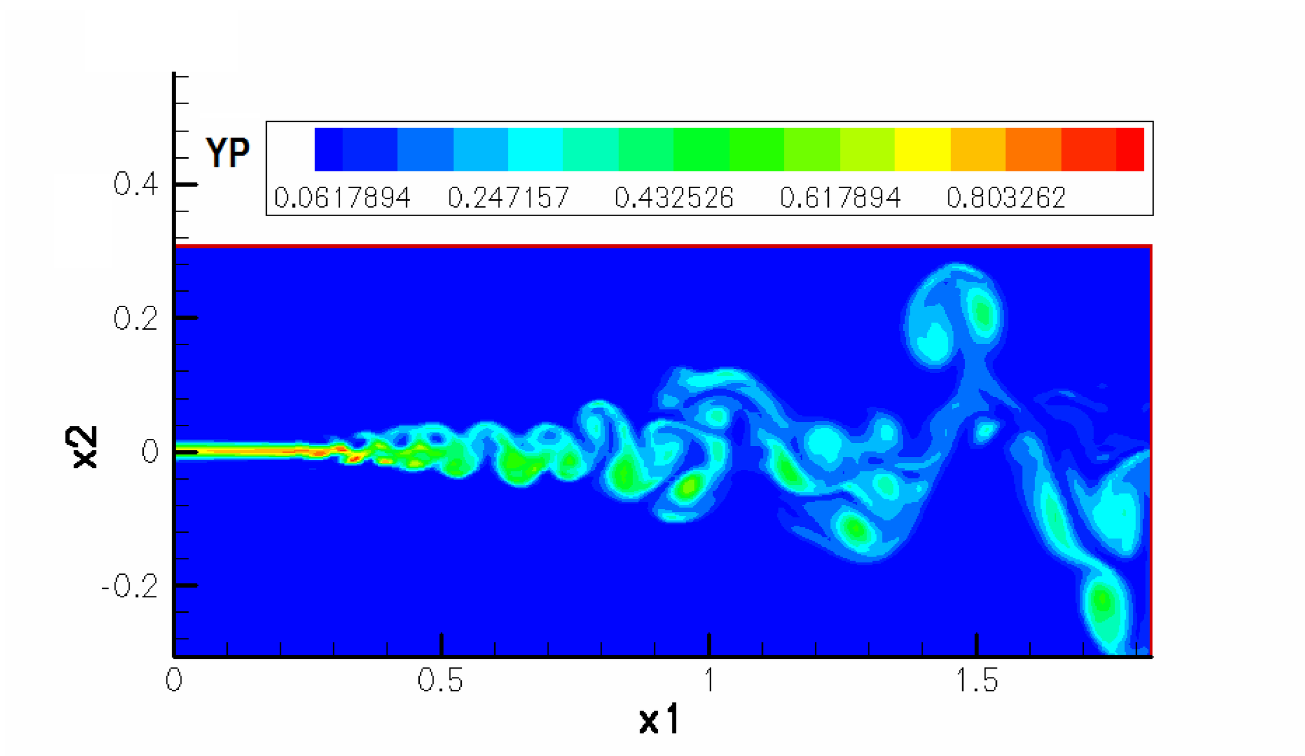
[Stencil not stable for very high resolutions]

Case 2 (stream wise and cross stream)
- **Implicit Fourth Order Accurate Tridiagonal Compact scheme**

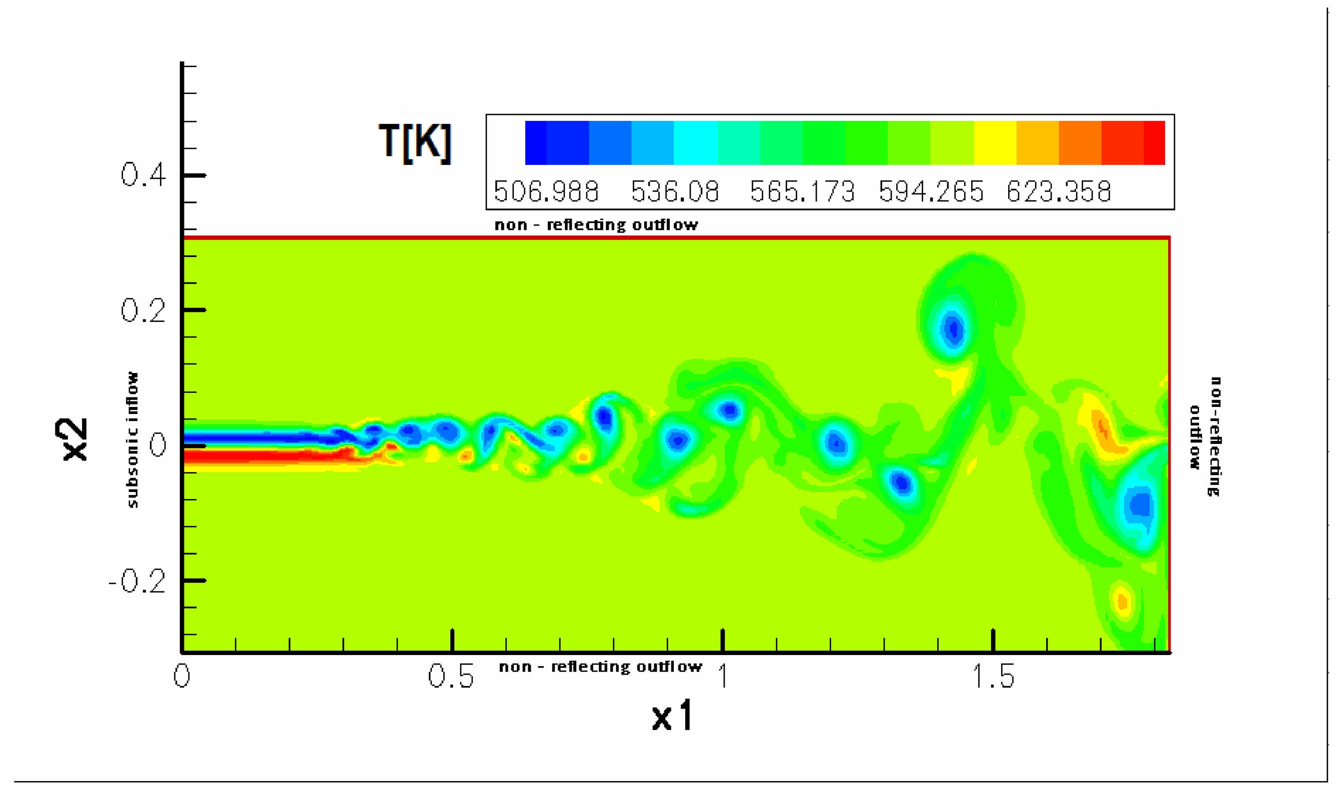
[*Stable Scheme but difficult to parallelize* **– Tridiagonal Solver Parallelized using Conjugate Gradient in PETSC – Scales linearly with the number of processors** *]

3. Grid Compression in cross stream (x_2) direction
4. $L_1=42\,D_{jet}, L_2=14\,D_{jet}, L_3=L_2$
5. Perturbations to Velocity in the inlet of the form $A\sin(2\pi f t+\phi)$
6. Parallelization of code using **Message Passing Interface** (MPI Fortran 77)

RESULTS



Contour of Product Mass Fraction



Contour of Temperature

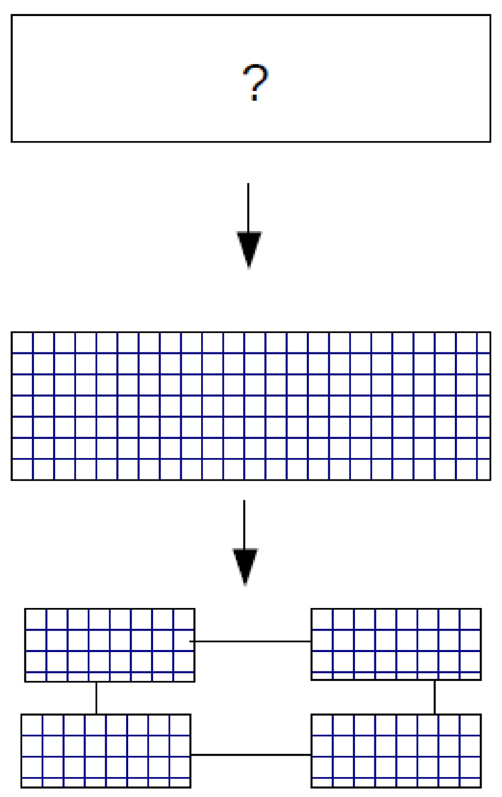
PROPOSED PARALLELIZATION

How do we solve the equations?
- We don't
- Solve *discrete* form of equations
- Use numerical methods

First step: Discretization of domain
- More grid points -> better solution

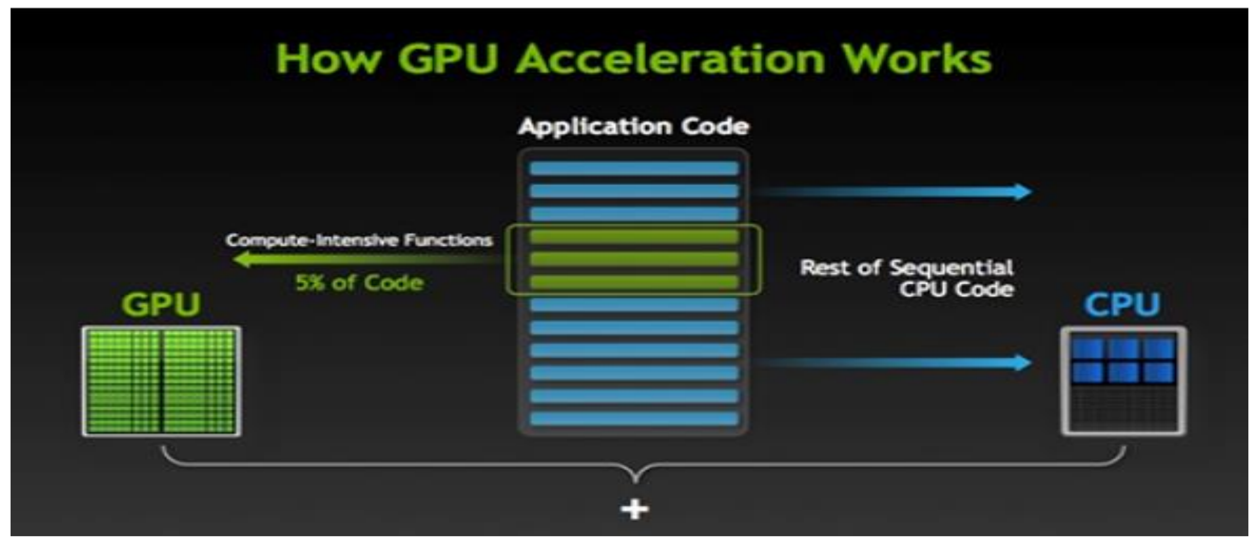
(more computation and memory required)

How do we handle large problems?
- Parallel Computing
- Distribution of problem among several Processors
- Every processor computers on 'its' part of the problem
- Processors need to communicate with each other



GRAPHICS PROCESSING UNITS (Next big thing in HPC)
- Massively parallel
- GPUs were designed to handle parallel data (think pixels)
- Each GPU consists of thousands of cores, each computing a small bit of data
- High computational power (peak performance on the order of Teraflops!)
- Clemson University Palmetto Cluster currently has > 500 GPUs and growing

A GPU has only ~ 5GB of memory, but our simulations are of order of Terabytes
- Use multiple GPUs!
- Two levels of parallelism
- Each GPU consists of hundreds of cores all computing in parallel
- Many GPUs work together in parallel to solve the problem



Challenges:
- GPUs are too fast!
- A naïve implementation will spend more time communicating data *between* GPUs than on computation itself
- Need to use better communication strategies
- Programming GPUs is more complex
- Need a good understanding of hardware
- Need to write a software that isn't irrelevant in a few months

Future Work

- Application of the numerical method (Stencil, Boundary Conditions, Initial Conditions) to high pressure combustion formulation with Real gas effects (improved models for heat / mass flux), Detailed reaction mechanism, Real gas equation of state (Cubic Peng Robinson)
- Validation and modification of Mixing Models used in LES, FDF and RANS by studying the conditional diffusion and scalar dissipation rate of the Jet.

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4. Yoo CS, Hong IM, "Characteristic bondary conditions for simulations of compressible reacting flows with multi-dimensional viscous and reaction effects", Combustion Theory and Modelling, 2006
5. Sankaran R, "Accelerating the Computation of Detailed Chemical Reaction Kinetics for Simulating Combustion of Complex Fuels", Cray Technical Workshop, ORNL, 2012