SAND2010-0740C

Computations of Chemically Reacting Flow

Habib N. Najm

Sandia National Laboratories
Livermore, CA

BES-NERSC Workshop, Washington DC, 2/9-10/2010

Overview

- Collaborators:
  - J. Prager, B. Debusschere, J. Ray, C. Safta — Sandia National Labs
  - M. Valorani, Univ. of Rome
  - D. Goussis, Nat. Tech. Univ. of Athens
  - O. Knio, Johns Hopkins Univ.
  - M. Frenklach, UC Berkeley
- Goal: Advance understanding of chemically reacting flows
- Approach:
  - Development of efficient algorithms and codes for multdimensional low Mach number reacting flow computations and analysis
  - Computational studies of low Mach number reacting flow with detailed chemical kinetics
  - Development of validated reduced chemical models

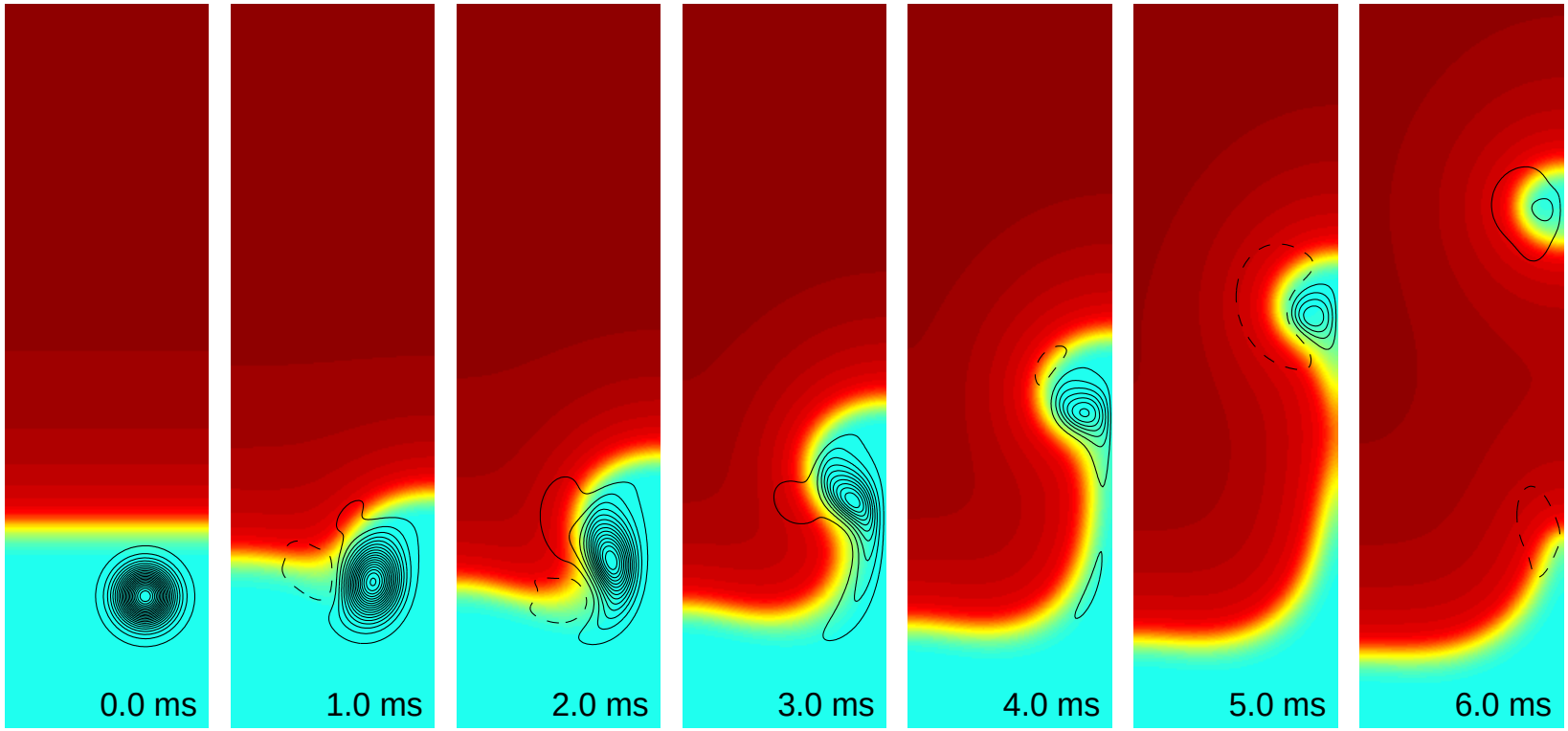
Science Objectives for the Next 3-5 Years

- Study the structure and dynamics of
  - Edge flames
  - Lifted laminar jet flames
- Address fuels over a range of complexity
  - Methane, nHeptane, isoOctane
- Examine dependence of flame structure/dynamics on mixture composition and flow details
- Experimental comparisons

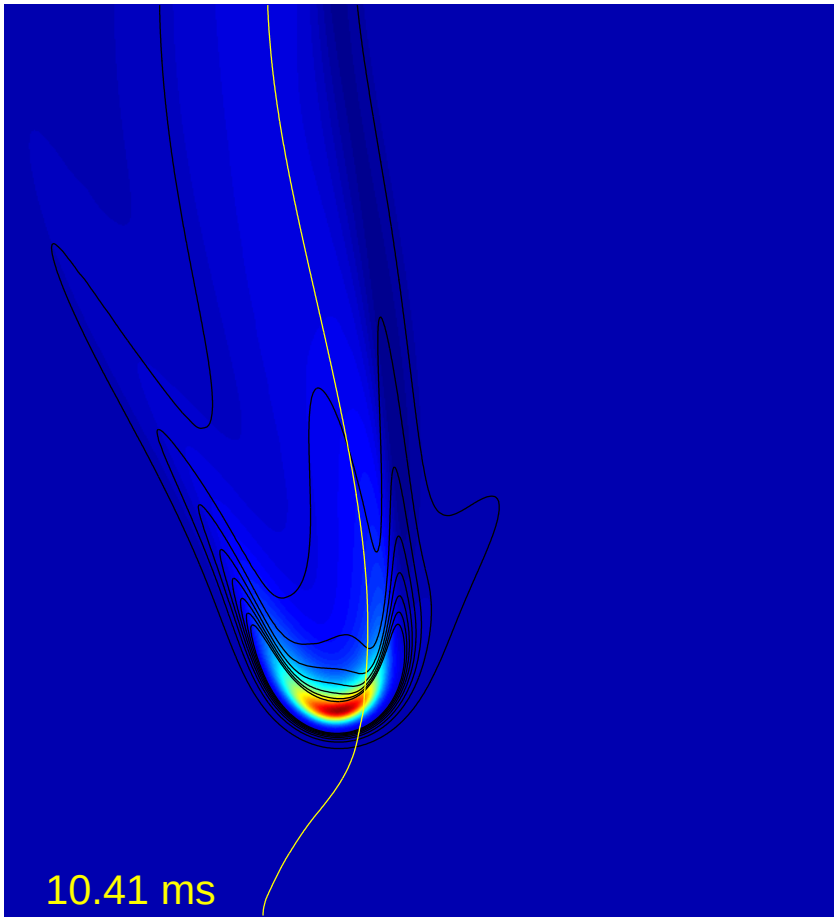
Computational Challenges in low Mach Number Reacting Flow Modeling

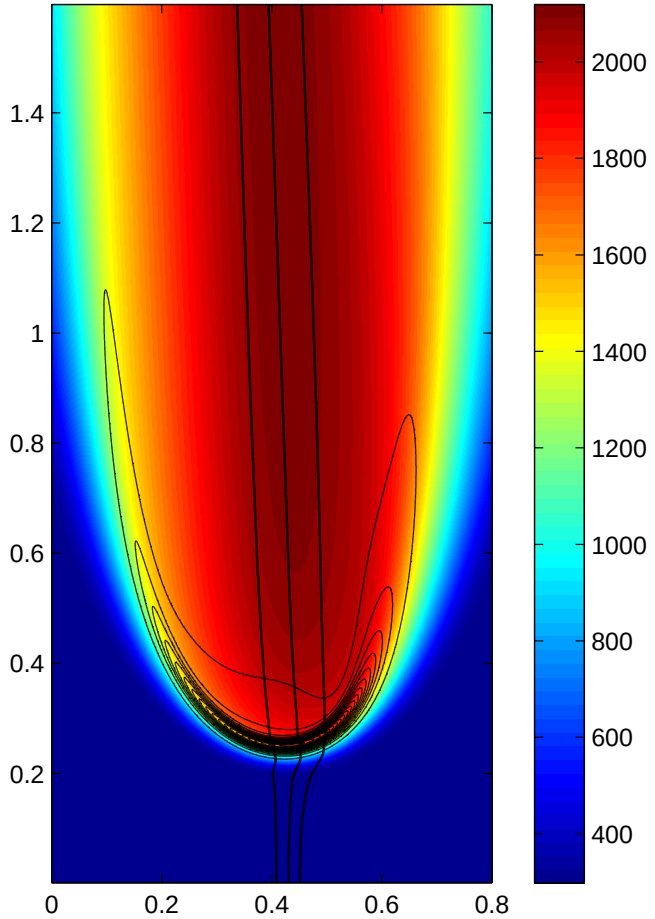
- Large range of length scales
  - Combustion system size $\mathcal{O}$(0.01–10) m
  - Internal flame structures $\mathcal{O}(100)\mu$m
  - Turbulence length scales
    - on the order of flame length scales at high Re
- Large range of time scales
  - Flow time scales can be slow: $\mathcal{O}$(10) ms
  - Fast chemical time scales: $\mathcal{O}$(1) ns
- Chemical model complexity
  - Methane-air $\sim$ 53 sp
  - nHeptane-air $\sim$ 560 sp
  - isoOctane-air $\sim$ 870 sp
- Multiphase, Radiation, Turbulence

Flame Vortex Interaction



Edge Flames


10.41 ms


1.4
1.2
1
0.8
0.6
0.4
0.2
0
0.2
0.4
0.6
0.8
2000
1800
1600
1400
1200
1000
800
600
400

Dimensionless Low Mach Number Equations

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \boldsymbol{v}) = 0$$

$$\frac{\partial (\rho \boldsymbol{v})}{\partial t} + \nabla \cdot (\rho \boldsymbol{v}\boldsymbol{v}) = -\nabla p + \frac{1}{\mathrm{Re}} \nabla \cdot \left\{ \mu [(\nabla \boldsymbol{v}) + (\nabla \boldsymbol{v})^T] - \frac{2}{3} \mu (\nabla \cdot \boldsymbol{v}) \mathbf{U} \right\}$$

$$\rho c_p \frac{DT}{Dt} = \frac{(\gamma - 1)}{\gamma} \frac{dp_o}{dt} + \frac{1}{\mathrm{RePr}} \nabla \cdot (\lambda \nabla T) - \frac{\rho}{\mathrm{ReSc}} \sum_{i=1}^{N} c_{p,i} \boldsymbol{V}_i \cdot \nabla T - \mathrm{Da} \sum_{i=1}^{N} h_i w_i$$

$$\frac{\partial (\rho Y_i)}{\partial t} + \nabla \cdot (\rho \boldsymbol{v} Y_i) = -\frac{1}{\mathrm{ReSc}} \nabla \cdot (\rho Y_i \boldsymbol{V}_i) + \mathrm{Da}\, w_i \qquad i = 1, \ldots, N$$

$$p_o = \frac{\rho T}{\overline{W}}$$

- Low Mach No., no body forces, bulk viscosity, or radiation
- Ideal gas, neglect Soret & Dufour effects — $\mathbf{U}$ is the unit tensor

Time Integration of Multi-D Low M Reacting Flow

- Density and Species update

$$\frac{\partial \rho}{\partial t} = \rho\left(-\frac{1}{T}\frac{\partial T}{\partial t} - \overline{W}\sum_{i=1}^{N}\frac{1}{W_i}\frac{\partial Y_i}{\partial t}\right)$$

$$\frac{\partial(\rho Y_i)}{\partial t} = -\nabla\cdot(\rho \boldsymbol{v} Y_i) - \frac{1}{\mathrm{ReSc}}\nabla\cdot(\rho Y_i \boldsymbol{V}_i) + \mathrm{Da}\ w_i \qquad i = 1,\ldots,N$$

- Projection scheme solution for $\boldsymbol{v}$

$$\frac{\partial(\rho\hat{\boldsymbol{v}})}{\partial t} = -\nabla\cdot(\rho\boldsymbol{v}\boldsymbol{v}) + \nabla\cdot\left\{\mu[(\nabla\boldsymbol{v}) + (\nabla\boldsymbol{v})^T] - \frac{2}{3}\mu(\nabla\cdot\boldsymbol{v})\mathbf{U}\right\}$$

$$\nabla^2 p = \frac{1}{\Delta t}\left[\nabla\cdot(\rho\hat{\boldsymbol{v}}) + \frac{\partial\rho}{\partial t}\right]; \qquad \rho\boldsymbol{v} = \rho\hat{\boldsymbol{v}} - \Delta t\nabla p$$

- Alternate constructions
  - (T, Y_i) rather than $(\rho, \rho Y_i)$ update
  - $\boldsymbol{v}$ rather than $(\rho\boldsymbol{v})$ projection

Time Integration of Stiff PDEs

- Species and energy conservation equations

$$\frac{\mathrm{d}u}{\mathrm{d}t} = C + D + R$$

- Explicit: Stiffness necessitates ~ 1 ns time steps
- Implicit:
  - Ok w/stiffness, but no need for implicit convection
- IMEX: Additive Implicit R, Explicit $C + D$
  - Deals well with chemical stiffness
  - Challenged by explicit diffusional stability
- Operator-Split: $C_{\Delta t/2} D_{\Delta t/2} R_{\Delta t} D_{\Delta t/2} C_{\Delta t/2}$
  - Explicit C
  - Explicit Runge Kutta Chebyshev (RKC) D
  - Implicit R

Computational Performance – NERSC Franklin

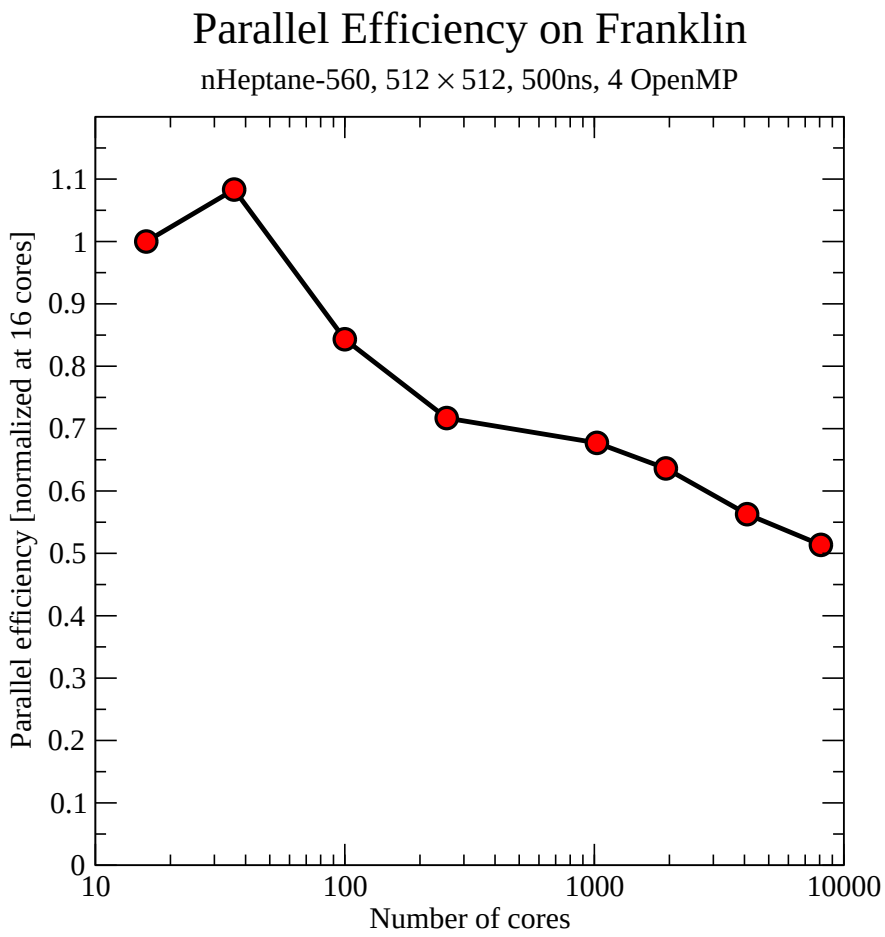
Cray XT4; 9,532 compute nodes; 2.3 GHz quad-core AMD Opt.

CPU Time per time step, 512$\times$512 mesh, 100 cores:

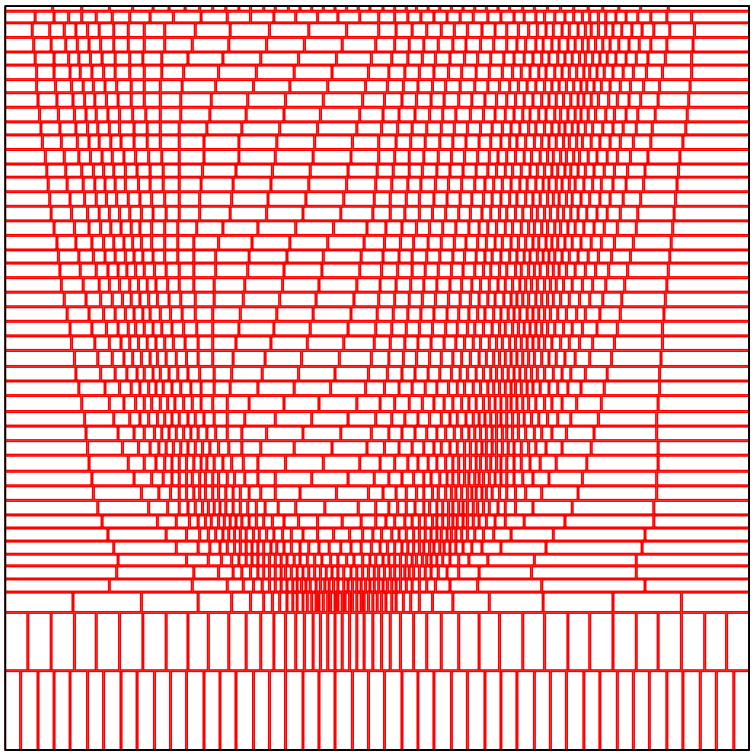
Mech	Parallelism	LINPACK	LAPACK	LAPACK^{opt}	LAPACK$^{opt}_{nJ}$
M560	MPI/OpenMP	198 min	53 min	22 min	37 min
	MPI only	–	–	25 min	37 min
M139	MPI/OpenMP	79 sec	90 sec	56 sec	121 sec
	MPI only	–	–	67 sec	120 sec
M66	MPI/OpenMP	20 sec	21 sec	17 sec	33 sec
	MPI only	–	–	22 sec	33 sec

Scalability – NERSC Franklin

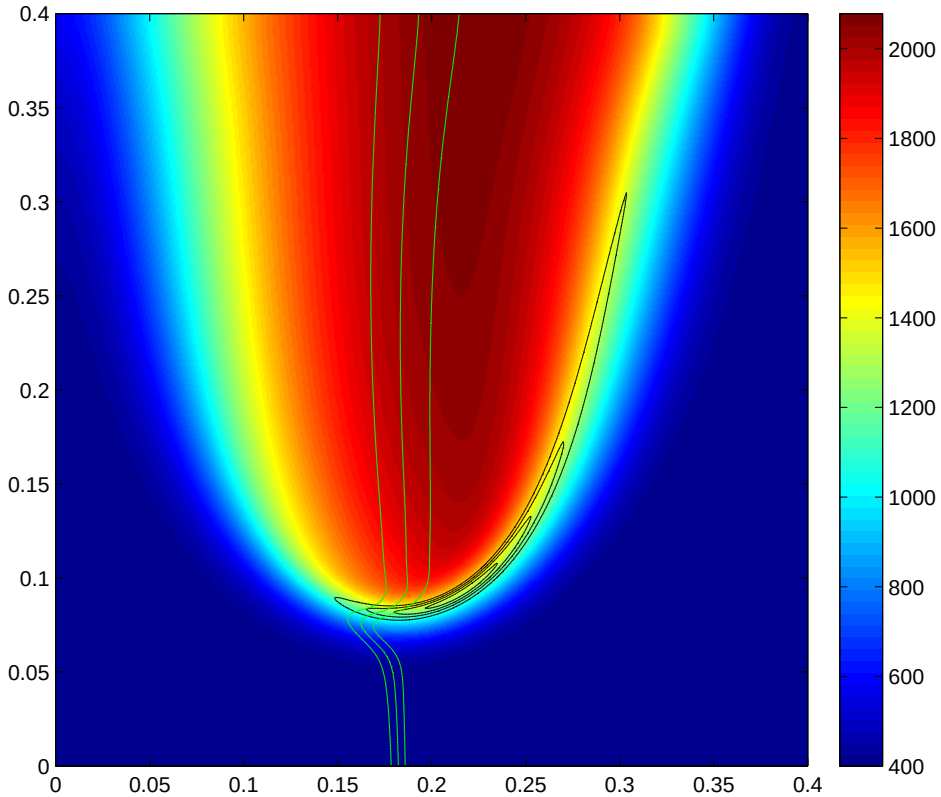
- 2D nHeptane edge flame
- 560 species, 2538 rxns
- Fixed 512×512 mesh
- 51% parallel efficiency on 8000 cores



nHeptane Edge Flame – M560 – NERSC Franklin



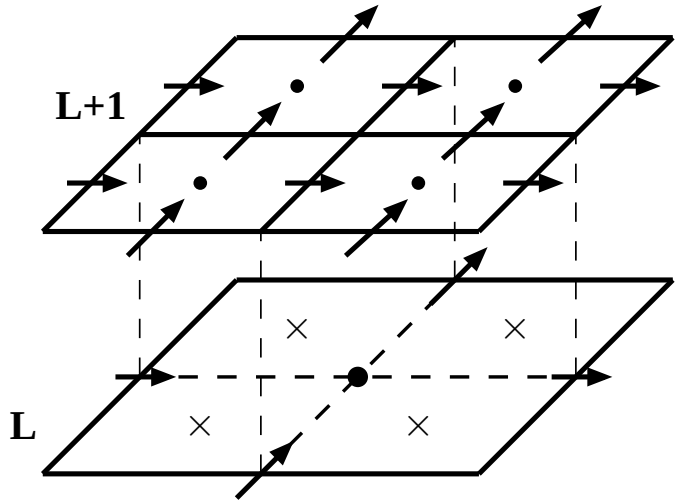
Domain Decomposition

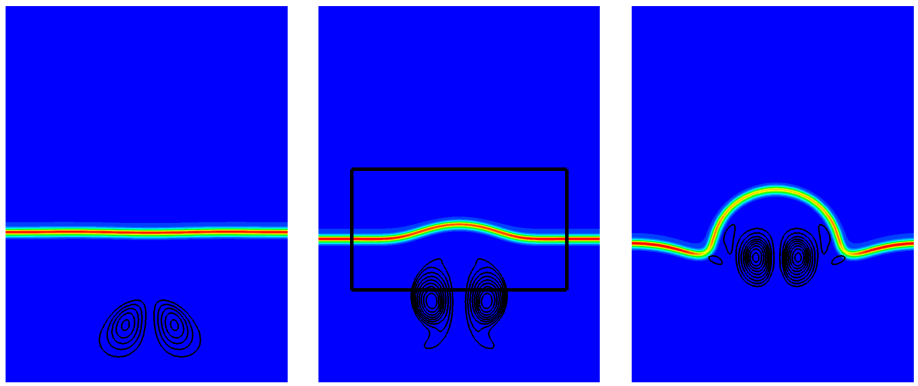


Global Flame Structure

Adaptive Mesh Refinement

- Structured mesh hierarchy
- Mesh libraries
  - Grace, Chombo
- High order spatial derivatives, interpolants, and filters
- Fourth-order low Mach reacting flow construction





Current HPC Requirements — Franklin

- Typical problems
  - Methane-air premixed flame-vortex
  - nHeptane edge flame
- # cores: 500-2000
- Aggregate Memory : 24 GB
- I/O per Run: 20 GB, 6 GB checkpoint files
- On-Line Storage: 30 GB
- Software and Services:
  - DVODE/sundials, LAPACK, hypre, Chombo, NERSC Consulting, craypat
- Data Transfer: 80 GB/yr

Current HPC Requirements — Primary codes

- **dflame**:
  - 2D uniform mesh finite-difference Fortran-77
  - 2^{nd}-order in space and time
  - Projection scheme for momentum equations
    FFT Poisson elliptic pressure solver
  - Operator Split implicit/explicit time integration
  - MPI+OpenMP parallelism
- **cfrfs**:
  - 2D Structured Adaptive mesh finite difference
    CCA + {C++, C, Fortran-77}
  - 4^{th}-order in space, 2^{nd} in time
  - Projection scheme for momentum equations
    hypre GMRES elliptic pressure solver
  - Operator Split implicit/explicit time integration
  - MPI parallelism

Current HPC Requirements — Limitations

- **dflame**:
  - Uniform mesh
  - 50% strong scalability at 8000 cores
    - Need to evaluate if/how this can be improved
- **cfrfs**:
  - MPI but no OpenMp
  - Dynamic load balancing is more challenging
  - Have yet to explore scalability in the O(10) K core range

Future HPC Requirements — 3-5 Years

- Methane/nHeptane/isoOctane edge and jet flames
- # cores: $\sim$ 100K
- 35M computational hrs
  - Presuming $\sim$ 60% parallel efficiency
- Aggregate Memory : 1-2 TB
- I/O per Run: 1-10 TB, 100-250 GB checkpoint files
- On-Line Storage: 3 TB
- Data Transfer: 10 TB/yr
- Archival Storage: 15 TB

Impact of 50$\times$ NERSC Resources Now

- For a given mesh size, and N species:
  - Memory $\propto N$
  - CPU $\propto N^2$
- $N_{\text{nHeptane}}/N_{\text{methane}} \sim 10$

Factor of 50 enables doing roughly the same methane flame with detailed nHeptane models

Enables parametric runs of laboratory-scale laminar flames with detailed nHeptane chemistry

However, we need to address parallel efficiency before we could go beyond $\mathcal{O}(10\ K)$ cores