Motivation

- Do we care problems with irregular dynamical memory access? YES.
  - Problems with localized error source benefit from adaptive nonuniform meshes
- Do we need this benchmark? YES.
  - Certain machines perform poorly on such problems
  - Parallel implementation may provide further performance improvement but is difficult:
    - load balancing / data (re)distribution
    - data dependence
    - false and true data sharing

Application Selection

- Representative of problem class relevant to scientific computing community
- Simple without sacrificing credibility and effectiveness
  - Stylized heat transfer problem
  - Can be load balanced for range of processor sets with little communication and remapping
  - Spectral Element Method (Patera)
  - Have irregular, dynamic memory accesses feature.
  - Adaptive Nonconforming Mesh

Heat Transfer Problem

- Mathematical model
  \[ \frac{\partial T}{\partial t} + V \cdot \nabla T = \varepsilon \nabla^2 T + S(x,t) \]
- Time splitting
  \[ \frac{T^{n+1} - T^n}{\Delta t} = -V \cdot \nabla T^n + S(x,t^n) \] 4th order R-K
  \[ Convexion \]
  \[ Diffusion \]

Heat Source Term

\[ s(x,t) = \begin{cases} 
\beta \left( \cos \left( \frac{\pi}{\alpha} \frac{x - x_0 - vt}{r} \right) + 1 \right) & \text{if } \|x-x_0-vt\| \leq \alpha \\
0 & \text{if } \|x-x_0-vt\| > \alpha 
\end{cases} \]
Spectral Element Method

- High-order weighted residual technique which combines
  - Geometrical flexibility of finite element method
  - High accuracy and rapid convergence of spectral method
- Variational form (GLL Quadrature)
  \[
  \left( \frac{T^m - \phi}{\Delta t}, \psi \right) = (\mathbf{B}(T^m), \mathbf{v})
  \]
- High order function expansion
  \[
  T_n(x, y, z) = \sum_{i=0}^{N} \sum_{j=0}^{N} \sum_{k=0}^{N} a_{ijk} \phi_i \phi_j \phi_k,
  \]
  \[
  \phi_i(x, y, z) = \hat{\phi}_i \mathbf{N}(x) \mathbf{N}(y) \mathbf{N}(z),
  \]

Base functions

\[
T_n(x, y, z) = \sum_{i=0}^{N} \sum_{j=0}^{N} \sum_{k=0}^{N} a_{ijk} \phi_i \phi_j \phi_k(x, y, z), \quad x, y, z \rightarrow \xi, \eta, \zeta \in [-1, 1]
\]

\[
h_{ij}^m(\xi) = \begin{cases} 
1 & \text{if } \xi = \xi_j \\
\frac{1}{N(N+1)} & \text{if } \xi = \xi_i \\
\frac{1}{N(N+1)} (1-\xi_i)(1-\xi_j) & \text{if } \xi \neq \xi_i, \xi_j 
\end{cases} 
\]

\[
\xi \in [-1, 1] \quad \forall q \in \{0, \ldots, N\}
\]

\[
\xi_q \text{ is } q\text{th GLL collocation point}
\]

Elemental Discrete Equations

\[
\frac{d}{dt} \sum_{i=0}^{N} \sum_{j=0}^{N} \sum_{k=0}^{N} \left( \frac{\partial}{\partial t} \right)^2 \phi_i \phi_j \phi_k \partial_x^2 + \left( \frac{\partial}{\partial t} \right)^2 \phi_i \phi_j \phi_k \partial_y^2 + \left( \frac{\partial}{\partial t} \right)^2 \phi_i \phi_j \phi_k \partial_z^2 = 0
\]

\[
D_i = \frac{\partial h_i}{\partial \xi} \quad \forall i = \{0, \ldots, K\} \quad \forall i, j, k = \{0, \ldots, N\}
\]

Global Discrete Equations

\[
\sum_{i=0}^{N} \sum_{j=0}^{N} \sum_{k=0}^{N} \left( \frac{\partial}{\partial t} \right)^2 \phi_i \phi_j \phi_k \partial_x^2 + \left( \frac{\partial}{\partial t} \right)^2 \phi_i \phi_j \phi_k \partial_y^2 + \left( \frac{\partial}{\partial t} \right)^2 \phi_i \phi_j \phi_k \partial_z^2 = 0
\]

\[
\sum_{i=0}^{N} \sum_{j=0}^{N} \sum_{k=0}^{N} \phi_i \phi_j \phi_k \partial_x \partial_y \partial_z f = \int_{\Omega} \frac{\partial^2 f}{\partial t^2} \partial x \partial y \partial z
\]

Nonconforming mesh

- Why nonconforming: local area refinement
- What is nonconforming
- Problem raised by nonconforming mesh: Continuity across element boundary

Mortar Element Method

Introduces a new mortar trace space:
- Preserve local structure
- Decouple the local/global computation
- Efficient for parallel computation
- Degrees of freedom are located in
  - Element interior
  - Mortar elements
Mortar Elements

- Mortar Element Method
  - Solution on elements
    \[ T_\alpha(x, y, z) = \sum_{i=1}^{N} \sum_{j=1}^{N} T_{\alpha,ij}(x) h_i(x) h_j(y), \quad x, y, z \rightarrow r, s, t \in [-1, 1] \]
  - Solution on mortars
    \[ \phi(x, y, z) = \sum_{i=1}^{N} \phi_i(x) h_i(y), \quad x, y, z \rightarrow P, S \in [-1, 1] \]

Mortar collocation points on nonconforming edges

- Mortar collocation points on the top and right faces of element 3.

Continuity across nonconforming element interfaces

- \( C^0 \) continuity is replaced by two conditions:
  1. Vertex condition: the solution on an element vertex equals to the solution at the corresponding mortar point.
  2. \( L^2 \) condition: the solution difference between an element face and its related mortar elements is minimized in an integral sense.

\[ \int_{\Gamma^e} (T \mid_{\alpha^e} - \phi) \nu ds = 0 \]
\[ \forall l = 1, ..., 4 \quad \forall y \in P_{l+1}(\Gamma^e) \]

Mapping for Nonconforming Faces

- Mapping direction from element to mortar.

Discrete Equations

- Conforming
  \[ A_{T_{l+1}} = B_{T_{l+1}} \]

- Nonconforming
  \[ \theta^T A_{T_{l+1}} = \theta^T B_{T_{l+1}} \]

Where \( \theta \) refers to Global transformation matrix assembled using local transformation matrix Q.

- Symmetrical
- Positive definite

Solved by CG with a Diagonal Preconditioner.

Mortar collocation points on nonconforming edges

- Nonconforming edge corresponding to the top face of element 3.

Mapping for Nonconforming Faces

- For reverse mapping from element to mortar.
Mesh Adaptation Procedure
- Perform adaptation every \( m \) time steps
- Refine elements close to high error region: elements have overlap with the heat source
- Coarsen the grid elsewhere if possible

Mesh Adaptation Restrictions
- The maximal refinement levels/the minimal element size
- Neighboring elements can not differ by more than one level of adaptation.

Adaptation in 3-D (h-type)

Time stepping procedure
- Move the source
  - Convection (RK4)
  - Diffusion (PCG)
- Step mod \( m = 0 \) ?
  - No
  - Yes
    - Mesh adaptation
    - Solution interpolation

Sample problem

Initial & Boundary condition
- Initial grid \([0,1]^3\)
- Initial temperature \( T=0 \)
- Initial heat source location \((0.30,0.28,0.28)\)
- Heat source strength \( \beta = 10 \)
- Heat source movement / Velocity field \( \mathbf{v} = (1,1,1) \)
- Boundary condition: \( T=0 \) @ all faces
Problem parameters and Verification

\[ \int \! \! \! \int \Delta \Omega \] At the last time step

<table>
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<th>( R_{max} )</th>
<th>( \Delta t )</th>
<th>( \alpha )</th>
<th>Adaptation interval</th>
<th>Step size</th>
<th># of elements</th>
<th>( \int ! ! ! \int \Delta \Omega )</th>
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Current Status

- Benchmark Design: http://www.nas.nasa.gov/Software/NPB
- Sequential implementation:
  - under construction
- Parallel implementation:
  - Space filling curve to handle the load balance

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