Unstructured Adaptive Meshes: Bad for your Memory?

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Background

- NAS Parallel Benchmarks (NPB, 1991)
  http://www.nas.nasa.gov/Software/NPB

benchmark problems		kernels					CFD app.			new benchmark
		CG	EP	IS	MG	FT	LU	SP	BT	UA
memory access	irregular	✓		✓						✓
	dynamic			✓						✓
scientific app.		✓			✓	✓	✓	✓	✓	✓

- Lack in the area of irregular and dynamically changing memory access

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

$$\frac{\partial T}{\partial t} + \mathrm{V} \bullet \vec{\nabla} T = \varepsilon \nabla^2 T + S(\mathbf{x},t)$$

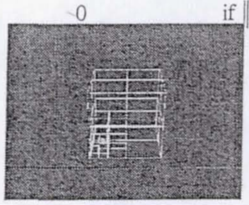
- Time splitting

Convection $\quad \dfrac{\hat{T} - T^n}{\Delta t} = -\mathrm{V} \bullet \vec{\nabla} T^n + S(\mathbf{x}, t^n) \quad$ *4th order R-K*

Diffusion $\quad \dfrac{T^{n+1} - \hat{T}}{\Delta t} = \varepsilon \nabla^2 T^{n+1} \quad$ *Euler implicit*

Heat Source Term

$$s(\mathbf{x},t) = \begin{cases} \beta\left(\cos\left(\pi \dfrac{\|\mathbf{x} - \mathbf{x}_0 - \mathbf{v}t\|}{\alpha}\right) + 1\right) & \text{if } \|\mathbf{x} - \mathbf{x}_0 - \mathbf{v}t\| \le \alpha \\ 0 & \text{if } \|\mathbf{x} - \mathbf{x}_0 - \mathbf{v}t\| > \alpha \end{cases}$$



Spectral Element Method

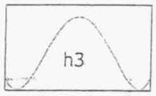
- High-order weighted residual technique which combines
  - Geometrical flexibility of finite element method
  - High accuracy and rapid convergence of spectral method
- Variational form (GLL Quadrature)

$$\left(\frac{T^{n+1}-\hat{T}}{\Delta t}, v\right) = (\varepsilon \bar{\nabla} T^{n+1}, \bar{\nabla} v)$$

- High order function expansion

$$T_h(x,y,z) = \sum_{i=0}^{N}\sum_{j=0}^{N}\sum_{k=0}^{N} T_{ijk}^{l} h_i(r) h_j(s) h_k(t), \quad x,y,z \to r,s,t \in [-1,1]$$

Base functions



$$T_h(x,y,z) = \sum_{i=0}^{N}\sum_{j=0}^{N}\sum_{k=0}^{N} T_{ijk}^{l} h_i(r) h_j(s) h_k(t), \quad x,y,z \to r,s,t \in [-1,1]$$

$$h_q(\xi) = \begin{cases} 1 & \text{if } \xi = \xi_q \\ -\dfrac{1}{N(N+1)L_N(\xi_q)} \dfrac{(1-\xi^2)L_N'(\xi)}{\xi - \xi_q} & \text{if } \xi \neq \xi_q \end{cases}$$

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

ξ_q is qth GLL collocation point

Elemental Discrete Equations

$$\varepsilon |J'| \sum_{m=0}^{N}\sum_{n=0}^{N}\sum_{o=0}^{N} \Big((\frac{2}{L_x^l})^2 \rho_n \rho_o \sum_{p=0}^{N} \rho_p D_{pi} D_{pm} \delta_{jn} \delta_{ko} +$$
$$(\frac{2}{L_y^l})^2 \rho_m \rho_o \sum_{p=0}^{N} \rho_p D_{pj} D_{pn} \delta_{im} \delta_{ko} +$$
$$(\frac{2}{L_z^l})^2 \rho_m \rho_n \sum_{p=0}^{N} \rho_p D_{pk} D_{po} \delta_{im} \delta_{jn} \Big) T_{mno}^l =$$
$$|J'| \sum_{m=0}^{N}\sum_{n=0}^{N}\sum_{o=0}^{N} \rho_i \rho_j \rho_k \delta_{im} \delta_{jn} \delta_{ko} f_{mno}^l$$

$$D_{ij} = \frac{dh_j}{d\xi}(\xi_i) \qquad \forall l = \{1,\ldots,K\} \qquad \forall i,j,k = \{0,\ldots,N\}^3$$

Global Discrete Equations

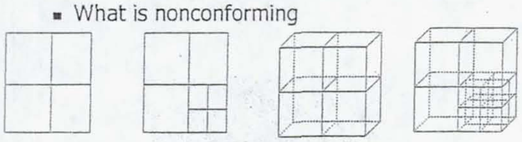
$$\varepsilon \Sigma' |J'| \sum_{m=0}^{N}\sum_{n=0}^{N}\sum_{o=0}^{N} \Big((\frac{2}{L_x^l})^2 \rho_n \rho_o \sum_{p=0}^{N} \rho_p D_{pi} D_{pm} \delta_{jn} \delta_{ko} +$$
$$(\frac{2}{L_y^l})^2 \rho_m \rho_o \sum_{p=0}^{N} \rho_p D_{pj} D_{pn} \delta_{im} \delta_{ko} +$$
$$(\frac{2}{L_z^l})^2 \rho_m \rho_n \sum_{p=0}^{N} \rho_p D_{pk} D_{po} \delta_{im} \delta_{jn} \Big) T_{mno}^l =$$
$$\Sigma' |J'| \sum_{m=0}^{N}\sum_{n=0}^{N}\sum_{o=0}^{N} \rho_i \rho_j \rho_k \delta_{im} \delta_{jn} \delta_{ko} f_{mno}^l \qquad f_h = \frac{T_h^{n+1} - \hat{T}_h^{n+1}}{\Delta t}$$

Σ' Stiffness summation

$$\Sigma' \bar{A}\bar{T} = \Sigma' \bar{B}\bar{\hat{T}} \to \quad AT = B\hat{T}$$

Nonconforming mesh

- Why nonconforming: local area refinement
- What is nonconforming



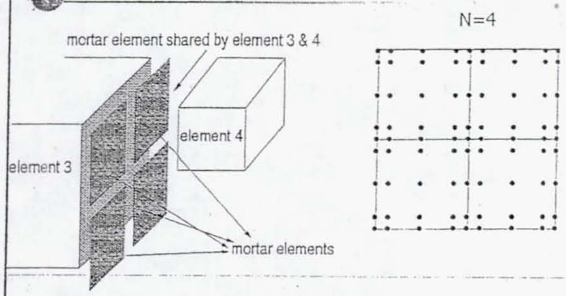
- Problem raised by nonconforming mesh: Continuity across element boundary

Mortar Element Method

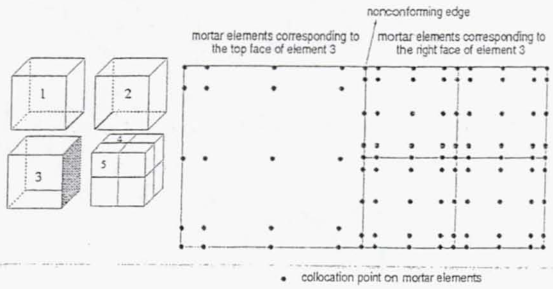
Introduces a new mortar trace space:

- 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 collocation points on nonconforming edges



Mortar Element Method

- Solution on elements

$$T_h(x,y,z)=\sum_{i=0}^{N}\sum_{j=0}^{N}\sum_{k=0}^{N}T^{l}_{ijk}h_i(r)h_j(s)h_k(t), \quad x,y,z\rightarrow r,s,t\in[-1,1]$$

- Solution on mortars

$$\phi(x,y,z)=\sum_{m=0}^{N}\sum_{n=0}^{N}\phi^{p}_{mn}h_m(\hat{r})h_n(\hat{s}), \quad x,y,z\rightarrow \hat{r},\hat{s}\in[-1,1]$$

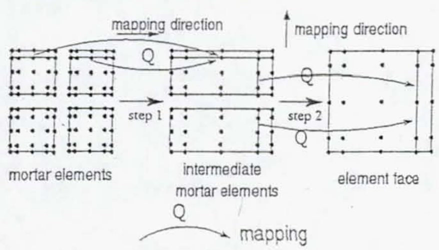
Continuity across nonconforming element iterfaces

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. $\int_{\Gamma^{k,l}}(T|_{\Omega^k}-\phi)\psi ds=0$

$$\forall l=1,\ldots,4 \;\; \forall\psi\in P_{N-2}(\Gamma^{k,l})$$

Mapping for Nonconforming Faces



Q^T For reverse mapping from element to mortar

Discrete Equations

conforming $\quad AT_h^{n+1}=B\hat{T}_h^{n+1}$

nonconforming $\quad \theta^T\bar{A}\theta T_h^{n+1}=\theta^T\bar{B}\hat{T}_h^{n+1}$

Where θ refers to Global transformation matrix assembled using local transformation matrix Q

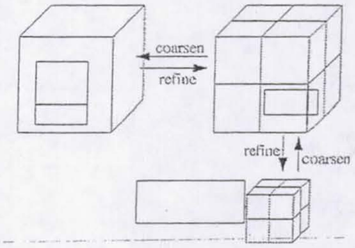
- symmetrical
- positive definite

Solved by CG with a Diagonal Preconditioner

Mesh Adaptation Procedure

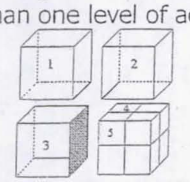
- Perform adaptation every m time steps
- Refine elements close to high error region: elements have overlap with the heat source
- Coarsen the grid elsewhere if possible

Adaptation in 3-D (h-type)

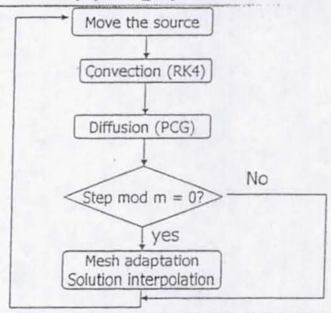


Mesh Adaptation Restrictions

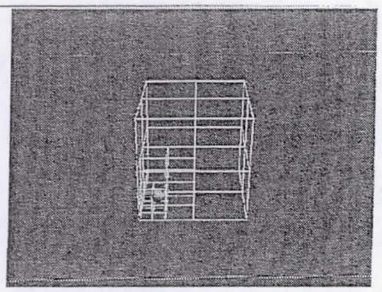
- The maximal refinement levels/the minimal element size
- Neighboring elements can not differ by more than one level of adaptation.



Time stepping procedure



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
  $v = (1,1,1)$
- Boundary condition: T=0 @ all faces

Problem parameters and Verification

$\int_{\Omega} T d\Omega$ At the last time step

class	R_{max}	Δt	α	Adaptation interval	Steps	# of elements	$\int_{\Omega} T d\Omega$
S	3	5.0E-2	0.04	40	50	120	2.7884126033740864E-4
W	4	2.5E-2	0.04	40	150	148	3.9507180536782076E-4
A	5	1.25E-3	0.06	35	150	554	6.6090402608961845E-4
B	6	6.25E-4	0.076	35	150	2010	6.7167313231442940E-4
C	7	3.125E-4	0.076	35	150	8079	3.3620548339346248E-4

Current Status

- Benchmark Design: http://www.nas.nasa.gov/Software/NPB
- Pencil and Paper Specification: 2/2003
- Sequential implementation:
  - under construction
- Parallel implementation:
  - Space filling curve to handle the load balance

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