

DG-FEM for PDE's Lecture 8

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A brief overview of what's to come

- Lecture I: Introduction and DG-FEM in ID
- Lecture 2: Implementation and numerical aspects
- Lecture 3: Insight through theory
- Lecture 4: Nonlinear problems
- Lecture 5: Extension to two spatial dimensions
- Lecture 6: Introduction to mesh generation
- Lecture 7: Higher order/Global problems
- Lecture 8: 3D and advanced topics

- \checkmark Let's briefly recall what we know
- ✓ Part I: 3D problems and extensions
 - Formulations and examples
 - Adaptivity and curvilinear elements
- ✓ Part II: The need for speed
 - ✓ Parallel computing
 - ✓ GPU computing
 - ✓ Software beyond Matlab

We are done with all the basics -- and we have started to see it work for us -- we know how to do

ID/2D problems
 Linear/nonlinear problems
 First and higher operators
 Complex geometries
 ... and we have insight into theory

All we need is 3D -- and with that comes the need for speed !

Extension to 3D?

It is really simple at this stage !

Weak form:

$$\int_{\mathsf{D}^k} \left[\frac{\partial u_h^k}{\partial t} \ell_n^k(\boldsymbol{x}) - \boldsymbol{f}_h^k \cdot \nabla \ell_n^k(\boldsymbol{x}) \right] \, d\boldsymbol{x} = -\oint_{\partial \mathsf{D}^k} \hat{\boldsymbol{n}} \cdot \boldsymbol{f}^* \ell_n^k(\boldsymbol{x}) \, d\boldsymbol{x},$$

Strong form:

$$\int_{\mathsf{D}^k} \left[\frac{\partial u_h^k}{\partial t} + \nabla \cdot \boldsymbol{f}_h^k \right] \ell_n^k(\boldsymbol{x}) \, d\boldsymbol{x} = \oint_{\partial \mathsf{D}^k} \hat{\boldsymbol{n}} \cdot \left[\boldsymbol{f}_h^k - \boldsymbol{f}^* \right] \ell_n^k(\boldsymbol{x}) \, d\boldsymbol{x},$$

$$\boldsymbol{f}^* = \{\{\boldsymbol{f}_h(\boldsymbol{u}_h)\}\} + \frac{C}{2} [\![\boldsymbol{u}_h]\!], \qquad C = \max_u \left|\lambda \left(\hat{\boldsymbol{n}} \cdot \frac{\partial \boldsymbol{f}}{\partial \boldsymbol{u}}\right)\right|,\$$

Nothing is essential new

Extension to 3D

Apart from the 'logistics' all we need to worry about is to choose our element and how to represent the solution

$$u(\mathbf{r}) \simeq u_h(\mathbf{r}) = \sum_{n=1}^{N_p} \hat{u}_n \psi_n(\mathbf{r}) = \sum_{i=1}^{N_p} u(\mathbf{r}_i) \ell_i(\mathbf{r}),$$

 $\mathbf{u} = \mathcal{V} \hat{\mathbf{u}}, \ \mathcal{V}^T \boldsymbol{\ell}(\mathbf{r}) = \boldsymbol{\psi}(\mathbf{r}), \ \mathcal{V}_{ij} = \psi_j(\mathbf{r}_i).$

We need points

$$N_p = \frac{(N+1)(N+2)(N+3)}{6},$$

We need an orthonormal basis

$$\psi_{ijk}(r,s,t) = 2\sqrt{2}P_i^{(0,0)}(a)P_j^{(2i+1,0)}(b)P_k^{(2i+2j+2,0)}(b)(1-b)^i(1-c)^{i+j},$$

Extension to 3D

For other element types, one simply need to define nodes and modes for that elements



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Extension to 3D

Everything is identical in spirit

Mass matrix $\mathcal{M}^k = J^k (\mathcal{V} \mathcal{V}^T)^{-1}.$

$$\mathcal{D}_r\mathcal{V}=\mathcal{V}_r, \ \ \mathcal{D}_s\mathcal{V}=\mathcal{V}_s, \ \ \mathcal{D}_t\mathcal{V}=\mathcal{V}_t,$$

Derivative

Diff matrix

$$\frac{\partial}{\partial x} = \frac{\partial r}{\partial x} \mathcal{D}_r + \frac{\partial s}{\partial x} \mathcal{D}_s + \frac{\partial t}{\partial x} \mathcal{D}_t,$$
$$\frac{\partial}{\partial y} = \frac{\partial r}{\partial y} \mathcal{D}_r + \frac{\partial s}{\partial y} \mathcal{D}_s + \frac{\partial t}{\partial y} \mathcal{D}_t,$$
$$\frac{\partial}{\partial z} = \frac{\partial r}{\partial z} \mathcal{D}_r + \frac{\partial s}{\partial z} \mathcal{D}_s + \frac{\partial t}{\partial z} \mathcal{D}_t,$$

Stiffness matrix

$$\mathcal{S}_r = \mathcal{M}^{-1} \mathcal{D}_r, \ \mathcal{S}_s = \mathcal{M}^{-1} \mathcal{D}_s, \ \mathcal{S}_t = \mathcal{M}^{-1} \mathcal{D}_t.$$

Example - Maxwell's equations

Consider Maxwell's equations

 $\varepsilon \partial_t E - \nabla \times H = -j, \qquad \quad \mu \partial_t H + \nabla \times E = 0,$

Write it on conservation form as

$$\frac{\partial q}{\partial t} + \nabla \cdot F = -J \quad F = \begin{bmatrix} -\hat{e} \times H \\ \hat{e} \times E \end{bmatrix} \quad q = \begin{bmatrix} E \\ H \end{bmatrix}$$

Represent the solution as

$$\Omega = \sum_{k} D^{k} \quad q_{N} = \sum_{i=1}^{N} q(\mathbf{x}_{i}, t) L_{i}(\mathbf{x})$$

and assume

$$\int_{D} \left(\frac{\partial \boldsymbol{q}_{N}}{\partial t} + \nabla \cdot \boldsymbol{F}_{N} - \boldsymbol{J}_{N} \right) L_{i}(\boldsymbol{x}) \, \mathrm{d}\boldsymbol{x} = \oint_{\partial D} L_{i}(\boldsymbol{x}) \hat{\boldsymbol{n}} \cdot [\boldsymbol{F}_{N} - \boldsymbol{F}^{*}] \, \mathrm{d}\boldsymbol{x}.$$





Example - Maxwell's equations

On each element we then define

$$\hat{M}_{ij} = \int_D L_i L_j \, \mathrm{d} \boldsymbol{x}, \quad \hat{S}_{ij} = \int_D \nabla L_j L_i \, \mathrm{d} \boldsymbol{x}, \quad \hat{F}_{ij} = \oint_{\partial D} L_i L_j \, \mathrm{d} \boldsymbol{x},$$

With the numerical flux given as

$$\hat{\boldsymbol{n}} \cdot [\boldsymbol{F} - \boldsymbol{F}^*] = \begin{cases} \boldsymbol{n} \times (\gamma \boldsymbol{n} \times [\boldsymbol{E}] - [\boldsymbol{B}]), \\ \boldsymbol{n} \times (\gamma \boldsymbol{n} \times [\boldsymbol{B}] + [\boldsymbol{E}]), \end{cases} \qquad [Q] = Q^- - Q^+$$

To obtain the local matrix based scheme

$$\hat{M}\frac{\mathrm{d}\hat{\boldsymbol{q}}}{\mathrm{d}t} + \hat{S}\cdot\hat{\boldsymbol{F}} - \hat{M}\hat{\boldsymbol{J}} = \hat{F}\hat{\boldsymbol{n}}\cdot[\hat{\boldsymbol{F}} - \hat{\boldsymbol{F}}^*],$$

One then typically uses an explicit Runge-Kutta to advance in time - just like ID/2D.

Apprications - Maxwell's equations

Simple wave propagation



An example - Maxwell's equations



An example - Maxwell's equations







Animations by Nico Godel (Hamburg)

Kinetic Plasma Physics







Introduction Deposition Particle Pushing Conclusions 0000000000 **Problem Statement and Notation** In hig Problem Statement and Notation effe Let $\Omega := \bigcup_i T_i$. Obtain E(x, t), H(x, t) on Ω by Maxwell's Equations Vlas $\partial_t E - \frac{1}{\varepsilon} \nabla \times H = -\frac{j}{\varepsilon},$ $\partial_t H + \frac{1}{\mu} \nabla \times E = 0,$ $\partial_t f$ Ma $\nabla \cdot H = 0, \quad \nabla \cdot E = \frac{\rho}{c}.$ Add particle distribution f(x, p, t) obeying the Vlasov Equation $\partial_t f + \mathbf{v} \cdot \partial_x f + q(E + \mathbf{v} \times B) \cdot \partial_p f = \langle \text{Sources} \rangle - \langle \text{Sinks} \rangle.$ Couple via $\rho := \int f \, dv, \qquad j := \int v f \, dv.$ Cc Andreas Klöckner Applied Mathematics, Bro

Wednesday, August 26, 2009 hods for High-Order Unstructured Particle-in-Cell Simulation

Particle-in-Cell (PIC) Methods

This is an attempt to solve the Vlasov/Boltzmann equation by sampling with P particles

$$f(x, p, t) = \sum_{n=1}^{P} q_n S(x - x_n(t)) \delta(p - p_n(t)),$$

$$\rho(x, t) = \sum_{n=1}^{P} q_n S(x - x_n(t)), \quad j(x, t) = \sum_{n=1}^{P} v_n q_n S(x - x_n(t))$$

Ideally we have

However, this is not practical, nor reasonable - so S(x) is a **shape-function**

Maxwell's equations

$$\varepsilon \partial_t E - \nabla \times H = -j, \quad \mu \partial_t H + \nabla \times E = 0,$$
$$\nabla \cdot (\varepsilon E) = \rho, \quad \nabla \cdot (\mu H) = 0,$$

Particle/Phase dynamics

$$\frac{dx_n}{dt} = v_n(t) \quad \frac{dmv_n}{dt} = q_n(E + v_n \times H) \quad m = \frac{1}{\sqrt{1 - (v_n/c)^2}}$$

Particles-to-fields

$$\rho(x,t) = \sum_{n=1}^{P} q_n S(x - x_n(t)), \quad j(x,t) = \sum_{n=1}^{P} v_n q_n S(x - x_n(t))$$

Fields-to-particles

$$E(x_n), H(x_n)$$

Some 3D results



Particle gun



Nothing special !

Everything you have done in ID/2D you can do in 3D in exactly the same way.

Linear/nonlinear problems
 First order/higher order operators
 Complex geometries

Further extensions

Adaptivity/non-conforming elements
 Curvilinear elements

Adaptivity/non-conformity

Question: Do element faces always have to match ?



Question: Can one use different order in each element?

Answer:Yes



Example - Adaptive solution

We consider a standard test case

$$\nabla^2 u(\mathbf{x}) = f(\mathbf{x}) \qquad u = 0, \mathbf{x} \in \partial \Omega$$

Domain is L-shaped

RHS so that the exact solution is

$$u(r,\theta) = r^{2/3}\sin(2\pi/3\theta)$$

Solution is singular !

Solved using full hp-adaptive solution







Example - Adaptive solution



Example - Adaptive solution - Maxwell's

 $\nabla \times \nabla \times \mathbf{E} + \omega^2 \mathbf{E} = \mathbf{f}, \mathbf{n} \times \mathbf{E} = 0, \mathbf{x} \in \Omega$







This is essential to fully benefit for complex problems



Figure 8.10: Snapshot of computed wave fields in the near-region of the solid surface-piercin cylinder. The cylinder surface is represented using a) a polygonal approximation and b) curvilinear approximation.

Example - Spherical Shallow Water equ

Dynamics of a thin layer of fluids on a sphere

$$\frac{\partial}{\partial t} \begin{bmatrix} \varphi \\ \varphi u \\ \varphi v \\ \varphi w \end{bmatrix} + \frac{\partial}{\partial x} \begin{bmatrix} \varphi u \\ \varphi u^2 + \frac{1}{2}\varphi^2 \\ \varphi uv \\ \varphi uv \\ \varphi uw \end{bmatrix} + \frac{\partial}{\partial y} \begin{bmatrix} \varphi v \\ \varphi vu \\ \varphi v^2 + \frac{1}{2}\varphi^2 \\ \varphi vw \end{bmatrix} + \frac{\partial}{\partial z} \begin{bmatrix} \varphi w \\ \varphi wu \\ \varphi wv \\ \varphi w^2 + \frac{1}{2}\varphi^2 \end{bmatrix} = \begin{bmatrix} 0 \\ -\frac{f}{a}(y\varphi w - z\varphi v) + \mu x \\ -\frac{f}{a}(z\varphi u - x\varphi w) + \mu y \\ -\frac{f}{a}(x\varphi v - y\varphi u) + \mu z \end{bmatrix}$$

$$\frac{\partial \overline{\varphi}}{\partial t} + \nabla \cdot \overline{F} = S(\overline{\varphi})$$

Stardard benchmark (Williamsson) in geophysical flow modeling

Example - Spherical Shallow Water equ



Example - Spherical Shallow Water equ



We have generalized everything to 3D

Linear/nonlinear problems
 First order/higher order operators
 Complex geometries
 Apaptivity
 Curvilinear elements

There is only one significant obstacle to solving large problems

SPEED !

✓ Let's briefly recall what we know

- ✓ Part I: 3D problems and extensions
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- Part II: The need for speed
 - Parallel computing
 - ✓ GPU computing
 - ✓ Software beyond Matlab

The need for speed !

So far, we have focused on 'simple' serial computing using Matlab based model.



The need for speed

Let us first understand where we spend the time





Test case is 3D Maxwells

The majority of work is local

The need for speed

The locality suggest that parallel computing will be beneficial

✓ Using OpenMP, the local work can be distributed over elements through loops.

✓ Using MPI the locality ensures a surface communication model.

Mixed OpenMP/MPI models also possible

 \checkmark A similar line of arguments can be used for iterative solvers.

Faffigien Serformance

# Processors	64	128	256	512
Scaled RK time	1.00	0.48	0.24	0.14
ldeal time	1.00	0.50	0.25	0.13

High performance is achieved through -

- Local nature of scheme
- Very Pure matrix-matrix operations
- Local bandwidth minimization
- ✓ Very efficient on-chip performance (~75%)

Challenges - ✓ Efficient parallel preconditioning

DG-FEM maps very well to classic multi-processor computing clusters and result in excellent speed-up.

... but such machines are expensive to buy and run.

Ex: To get on the Top500 list, requires about \$3m to purchase a cluster with 16-18Tflop/s performance.

What we need is supercomputing on the desktop

For FREE !

... or at least at a fraction of the price

CPUs vs GPUs



Notice the following



The memory bandwidth and the peak performance on Graphics cards (GPU's) is developing MUCH faster than on CPU's

At the same time, the mass-marked for gaming drives the prices down -- we have to find a way to exploit this !

But why is this ?

Target for CPU:

- Single thread very fast
- Large caches to hide latency
- Predict, speculate etc





Lots of very complex logic to predict behavior



But why is this ?

For streaming/graphics cards it is different

- Throughput is what matters
- Hide latency through parallelism
- Push hierarchy onto programmer

Much simpler logic with a focus on performance







GPUs 101



GPU layout



- ✓ I GPU = 30 MPs
- ✓ I MP has I IU, 8 SP, I DP
- ✓ I MP has I6KiB shared and 32 KiB Register memory
- √240 (512) threads
- ✓ Dedicated RAM at I40GB/s
- Limited caches





Gains	Losses
 Memory Bandwidth (140 GB/s vs. 12 GB/s) Compute Bandwidth (Peak: 1 TF/s vs. 50 GF/s, Real: 200 GF/s vs. 10 GF/s) 	 Recursion Function pointers Exceptions IEEE 754 FP compliance Cheap branches (i.e. ifs)

Already here it is clear that programming models/codes may have to undergo substantial changes -- and that not all will work well





Block (1,	0)		
Thread (0, 3)	Thread (1, 3)	Thread (2, 3)	Thread (3, 3)
Thread (0, 2)	$\frac{\text{Thread}}{(1,2)}$	Thread (2, 2)	Thread (3, 2)
Thread (0, 1)	$\frac{\textbf{Thread}}{(1,1)}$	Thread (2, 1)	Thread (3, 1)
Thread (0, 0)	$\begin{array}{c} \textbf{Thread} \\ (1,0) \end{array}$	Thread (2, 0)	Thread (3, 0)

Genuine multi-tiered parallelism
 Grids
 blocks
 threads

Only threads within a block can talk
 Blocks must be executed in order

Grids/blocks/threads replace loops

✓ Until recently, only single precision

✓ Code-able with CUDA (C^{BROWN} tension)





Memory model:





✓ Lots of multi-processors (about 30)
 ... communicate through global mem
 ✓ Registers, shared memory, and threads communicate with low latency

... but memory is limited (16-32 KiB)



GPUs 101



✓ Global memory (4GiB/PU) is plentiful

... but latency is high (512 bit bus) ... and stride one is preferred

✓ Texture is similar to global memory

... allows more general access patterns ... but it is read only

Туре	Per	Access	Latency
Registers	thread	R/W	1
Local	thread	R/W	1000
Shared	block	R/W	2
Global	grid	R/W	1000
Constant	grid	R/O	1-1000
Texture	grid	R/O	1000





Matrix transpose



Memory bandwidth will be a limit here



Using just global memory



Let's consider an example

Using just texture(read)+global(write) memory



Getting better

Let's consider an example

E III

Transpose block-by-block in shared memory - this does not care about strides



Let's consider an example



Additional improvements are possible for small matrices - bank conflicts in shared memory





As T. Warburton said in the his talk:

The CPU is mainly the traffic controller ... although it need not be

✓ The CPU and GPU runs asynchronously

✓ CPU submits to GPU queue

✓ CPU synchronizes GPUs

Explicitly controlled concurrency is possible



GPUs overview



- ✓ GPUs exploit multi-layer concurrency
- The memory hierarchy is deep
- Memory padding is often needed to get optimal performance
- Several types of memory must be used for performance

First factor of 5 is not too hard to get
 Next factor of 5 requires quite some work
 Additional factor of 2-3 requires serious work

So what does all this mean ?

✓ GPU's has deep memory hierarchies so local is good
The majority of DG operations are local

Compute bandwidth >> memory bandwidth
 High-order DG is arithmetically intense

✓ GPU global memory favors dense data
 ➡ Local DG operators are all dense

With proper care we should be able to obtain excellent performance for DG-FEM on GPU's







Nodes in threads, elements for blocks



Other choices: ✓D-matrix in shared, data in global (small N) ✓Data in shared, D-matrix is global (large N)





Where you need it most



Also in double precision

... and for larger and larger grids





Similar results for DG-FEM Poisson solver with CG



Note: No preconditioning



Combined GPU/MPI solution





Example - a Mac Mini







K=201765 elements 3rd order elements

Computation by N. Godel

Example: Military aircraft





	CPU global	29 h 6 min 46 s	1.0
	GPU global	39 min 1 s	44.8
K.	GPU multirate	11 min 50 s	147.6



Not just for toy problems

228K elements5th order elements78m DOF68k time-steps

Time ~ 6 hours



711.9 GFlop/s on one card

Computation by N. Godel

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2008

Beyond Maxwell's equations













Beyond Maxwell's equations



Speedup Factor

Speedup

2D Navier-Stokes test case



Want to play yourself ?



Code MIDG available at http://nvidia.com/cuda

Note: Single precision - double to come

Do we have to write it all ?

No :-)

Sook related codes - all at <u>www.nudg.org</u>

✓ Matlab codes

√NUDG++ - a C++ version of 2D/3D codes (serial)

In the second second

✓ MIDG - a bare bones parallel/GPU code for Maxwell's equations Other codes

✓ Slegde++ - C++ operator code. Interfaced with parallel solvers (Trilinos and Mumps) and support for adaptivity and non-conformity. Contact Lucas Wilcox (UT Austin/ICES)

✓ **deal.II** - a large code with support for fully non-conforming DG with adaptivity etc. Only for squares/cubes. <u>www.dealii.org</u>

✓ Nektar++ - a C++ code for both spectral elements/hp and DG. Mainly for CFD. Contact Prof Spencer Sherwin (Imperial College, London)

Progress ?



Year 2001

250k tets, 4th order 50m dof, 100k timesteps

24 hours on 512 procs

Year 2008

82k tets, 4th order 17m dof, 60k timesteps

Few hours on GPU



Thanks !

Many people have contributed to this with material, figures, examples etc

Tim Warburton (Rice University)
 Lucas Wilcox (UT Austin)
 Andreas Kloeckner (Brown)
 Nico Goedel (Hamburg)
 Hendrick Riedmann (Stuttgart)
 Francis Giraldo (NRL, Monterrey)

... and to you for hanging in there !