DGFEM 2012

DG-FEM for PDE's
Lecture 8

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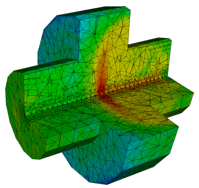
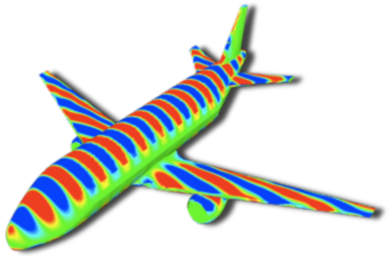




A brief overview of what's to come

- Lecture 1: Introduction and DG-FEM in 1D
- 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

Lecture 8

- ✓ 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

Lets summarize

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

- ✓ 1D/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

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

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

We need points

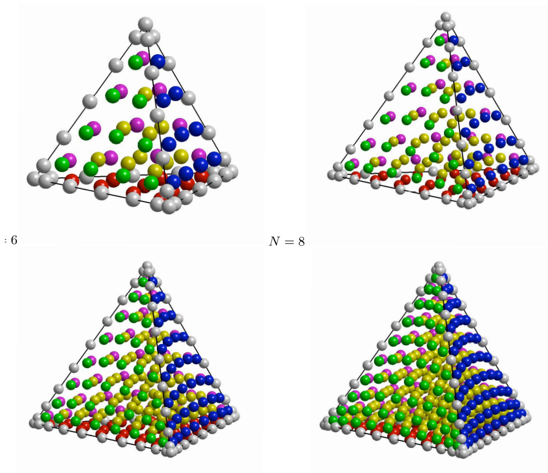
$$N_p = \frac{(N+1)(N+2)(N+3)}{6},$$

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



Extension to 3D

Everything is identical in spirit

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

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

Derivative

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

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

Example - Maxwell's equations

Consider Maxwell's equations

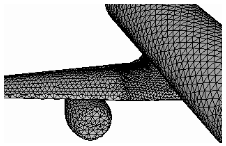
$$\varepsilon \partial_t E - \nabla \times H = -j, \qquad \mu \partial_t H + \nabla \times E = 0,$$

Write it on conservation form as

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

Represent the solution as

$$\Omega = \sum_k D^k \qquad q_N = \sum_{i=1}^{N} q(\mathbf{x}_i, t) L_i(\mathbf{x})$$



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

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

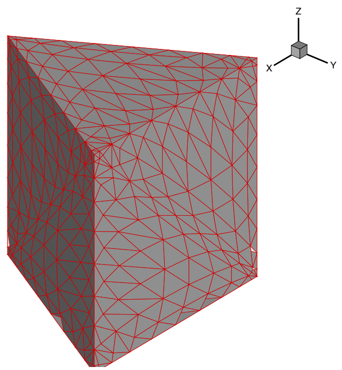
To obtain the local matrix based scheme

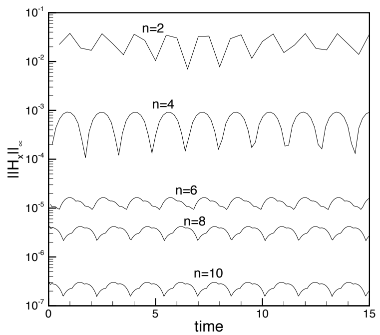
$$\hat{M} \frac{\mathrm{d}\hat{\boldsymbol{q}}}{\mathrm{d}t} + \hat{S} \cdot \hat{\boldsymbol{F}} - \hat{M}\hat{\boldsymbol{J}} = \hat{F} \hat{\boldsymbol{n}} \cdot [\hat{\boldsymbol{F}} - \hat{\boldsymbol{F}}^*],$$

One then typically uses an explicit Runge-Kutta to advance in time - just like 1D/2D.

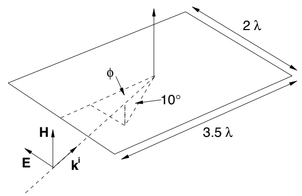
An example - Maxwell's equations

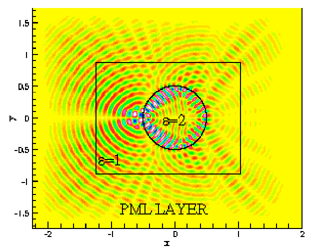
Simple wave propagation

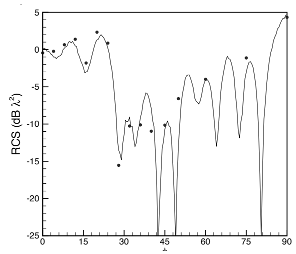


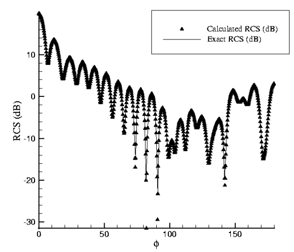


An example - Maxwell's equations

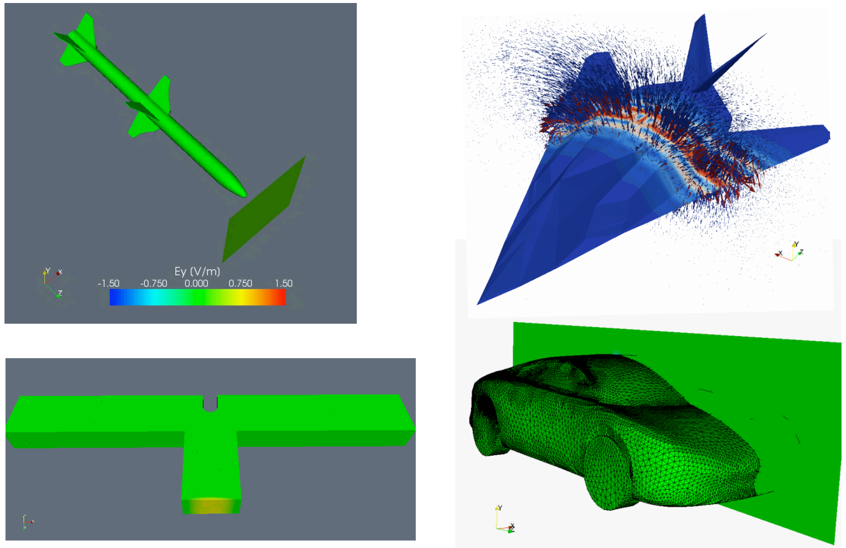








An example - Maxwell's equations

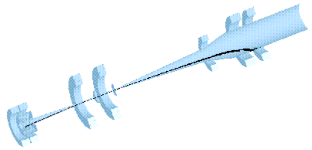


Animations by Nico Godel (Hamburg)

Kinetic Plasma Physics

Important applications

- ✓ High-power/High-frequency microwave generation
- ✓ Particle accelerators
- ✓ Laser-matter interaction
- ✓ Fusion applications, e.g., plasma edge
- ✓ etc



Kinetic Plasma Physics

In high-speed plasma problems dominated by kinetic effects, one needs to solve for f(x,p,t) - 6D+1

Vlasov/Boltzmann equation

$$\partial_t f + v \cdot \partial_x f + q(E + v \times B) \cdot \partial_p f = \langle \text{Sources} \rangle - \langle \text{Sinks} \rangle.$$

Maxwell's equations

$$\begin{aligned} \partial_t E - \frac{1}{\varepsilon} \nabla \times H &= -\frac{j}{\varepsilon}, \\ \partial_t H + \frac{1}{\mu} \nabla \times E &= 0, \\ \nabla \cdot H = 0, \qquad \nabla \cdot E &= \frac{\rho}{\varepsilon}. \end{aligned}$$

Coupled through $\rho := \int f \, dv, \qquad j := \int vf \, dv.$

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

$$S(x) = \delta(x) \longleftarrow \text{a point particle}$$

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

Particle-in-Cell Methods

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

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

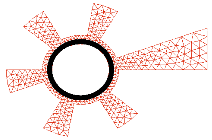
Particles-to-fields

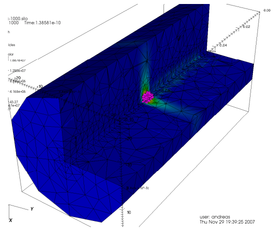
$$\rho(x,t) = \sum_{n=1}^{P} q_n S(x - x_n(t)), \quad j(x,t) = \sum_{n=1}^{P} v_n q_n S(x - x_n(t))$$

Fields-to-particles $E(x_n), H(x_n)$

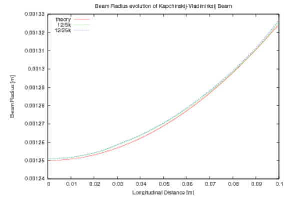
Kinetic Plasma Physics

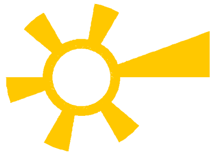
Magnetron modeling

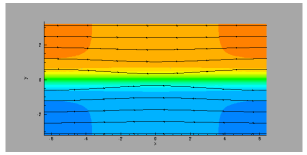




Linear accelerator

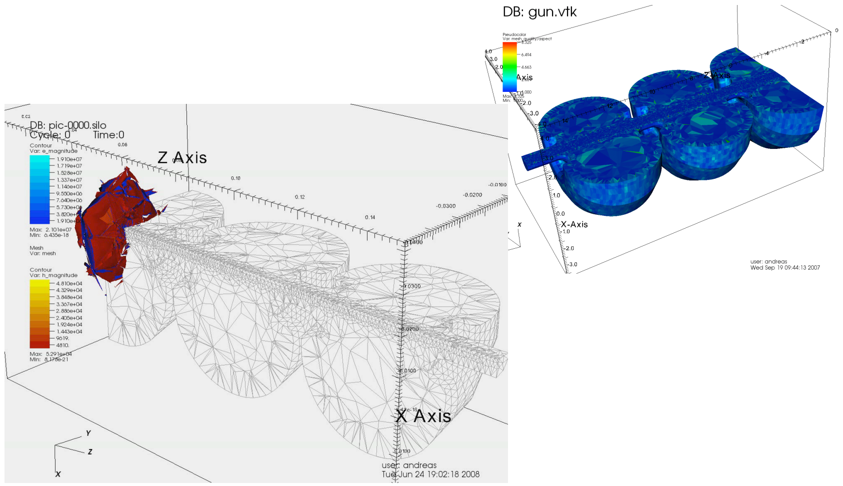






Magnetic reconnection

Particle gun



Compressible fluid flow

Time-dependent Euler equations

$$\frac{\partial \mathbf{q}}{\partial t} + \frac{\partial \mathbf{F}}{\partial x} + \frac{\partial \mathbf{G}}{\partial y} = 0,$$

$$\mathbf{q} = \begin{pmatrix} \rho \\ \rho u \\ \rho v \\ E \end{pmatrix}, \ \mathbf{F} = \begin{pmatrix} \rho u \\ \rho u^2 + p \\ \rho u v \\ u(E+p) \end{pmatrix}, \ \mathbf{G} = \begin{pmatrix} \rho v \\ \rho u v \\ \rho v^2 + p \\ v(E+p) \end{pmatrix}$$

- ✓ Gas
- ✓ High speed
- ✓ etc

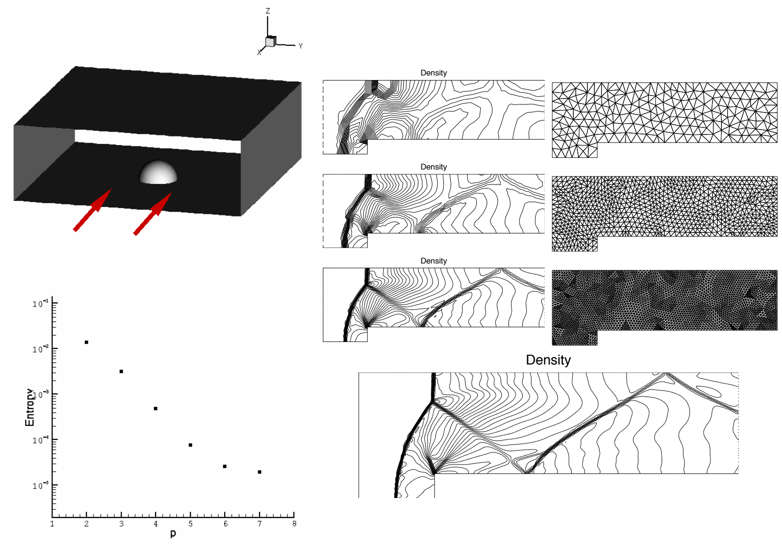
Formulation is straightforward

$$\int_{\mathsf{D}^k} \left(\frac{\partial \mathbf{q}_h}{\partial t}\phi_h - \mathbf{F}_h \frac{\partial \phi_h}{\partial x} - \mathbf{G}_h \frac{\partial \phi_h}{\partial y} \right) d\boldsymbol{x} + \oint_{\partial \mathsf{D}^k} (\hat{n}_x \mathbf{F}_h + \hat{n}_y \mathbf{G}_h)^* \phi_h d\boldsymbol{x} = 0.$$

$$(\hat{n}_x \mathbf{F}_h + \hat{n}_y \mathbf{G}_h)^* = \hat{n}_x \{\{\mathbf{F}_h\}\} + \hat{n}_y \{\{\mathbf{G}_h\}\} + \frac{\lambda}{2} \cdot [\![\mathbf{q}_h]\!].$$

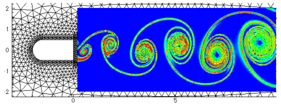
Challenge: Shocks -- this requires limiting/filtering

Compressible fluid flow

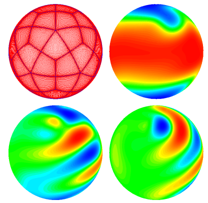


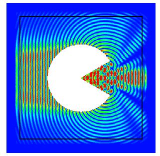
The list goes on ..

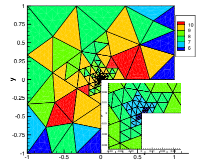
The same DG-FEM computation platform has been used for all examples and many other problem types



- ✓ Flow mixing and control
- ✓ Poisson/Helmholtz equations
- ✓ Shallow water flows on the sphere
- ✓ Adjoint based adaptive solution/design







3D Extension

Nothing special !

Everything you have done in 1D/2D you can do in 3D in exactly the same way.

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

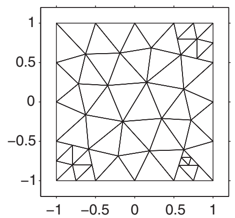
Further extensions

- ✓ Adaptivity/non-conforming elements
- ✓ Curvilinear elements

Adaptivity/non-conformity

Question: Do element faces always have to match ?

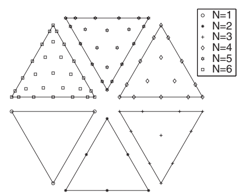
Answer: No



h-nonconform

Question: Can one use different order in each element ?

Answer:Yes



p-nonconform

Example - Adaptive solution

We consider a standard test case

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

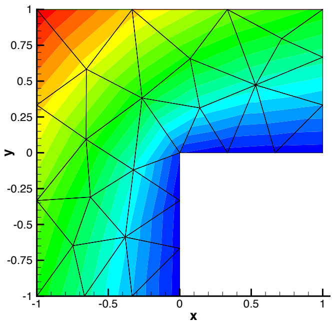
Domain is L-shaped

RHS so that the exact solution is

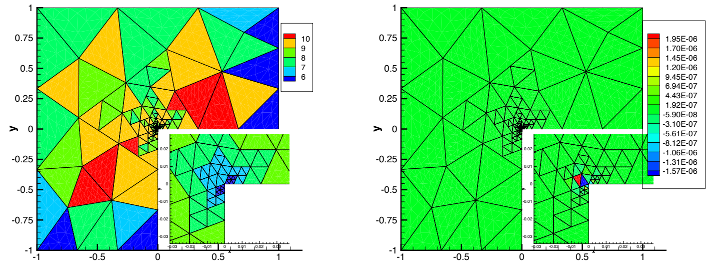
$$u(r,\theta) = r^{2/3}\sin(2\pi/3\theta)$$

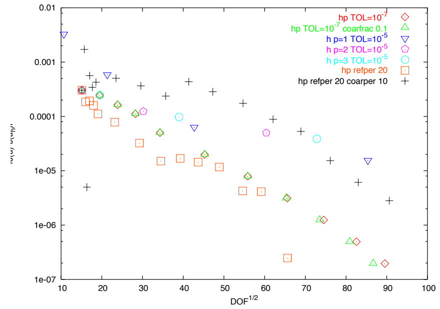
Solution is singular !

Solved using full hp-adaptive solution



Example - Adaptive solution

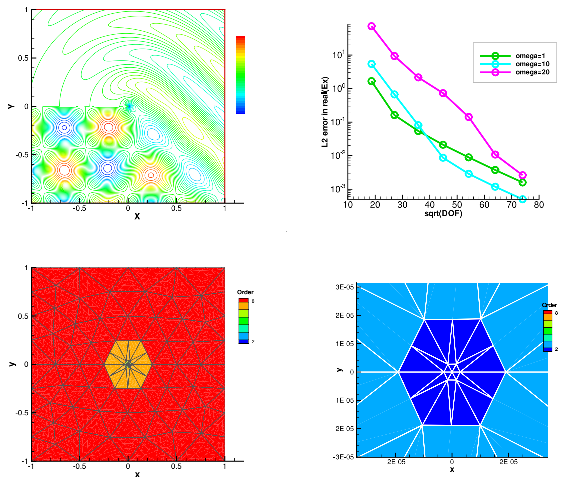




Spectral convergence even for a singular solution

Example - Adaptive solution - Maxwell's

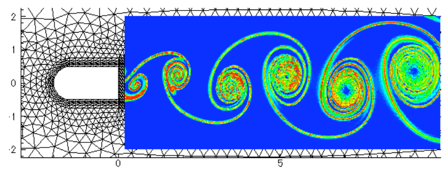
$$\nabla \times \nabla \times \mathbf{E} + \omega^2 \mathbf{E} = \mathbf{f}, \mathbf{n} \times \mathbf{E} = 0, \mathbf{x} \in \Omega$$

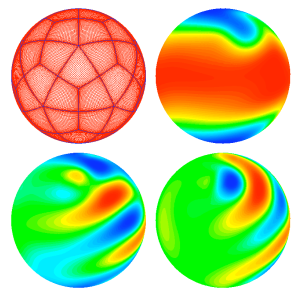


Curvilinear elements

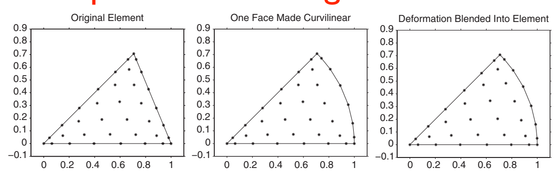
What: Elements that conform exactly to a curved boundary

Why: Accuracy !



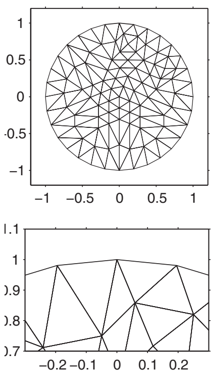


This is a unique feature to high-order elements



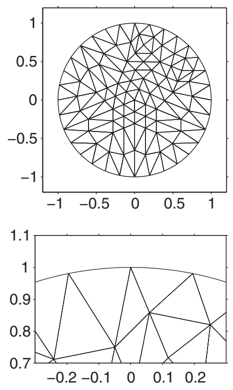
Example - Maxwell's equations

$$H^x(x,y,t=0)=0,\quad H^y(x,y,t=0)=0,$$
$$E^z(x,y,t=0)=J_6(\alpha_6 r)\cos(6\theta)\cos(\alpha_6 t),$$



N	h	$h/2$	$h/4$	Rate
1	1.09E-01	3.78E-02	8.96E-03	1.80
2	2.37E-02	2.70E-03	3.58E-04	3.02
3	5.77E-03	1.09E-03	2.70E-04	2.21
4	4.39E-03	1.09E-03	2.72E-04	2.01
5	4.38E-03	1.09E-03	2.72E-04	2.00
6	4.40E-03	1.09E-03	2.72E-04	2.01
7	4.41E-03	1.09E-03	2.73E-04	2.01

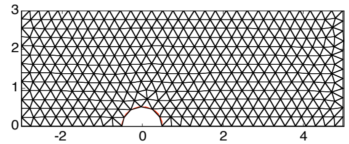
N	h	$h/2$	$h/4$	Rate
1	1.09E-01	3.78E-02	8.96E-03	1.80
2	2.21E-02	2.23E-03	2.05E-04	3.38
3	3.12E-03	1.92E-04	1.28E-05	3.97
4	6.01E-04	1.95E-05	5.88E-07	5.00
5	9.89E-05	1.69E-06	2.72E-08	5.92
6	1.74E-05	1.31E-07	9.81E-10	7.06
7	2.08E-06	8.97E-09	7.93E-11*	7.34*

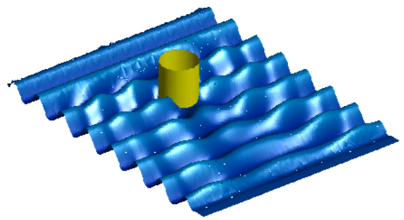


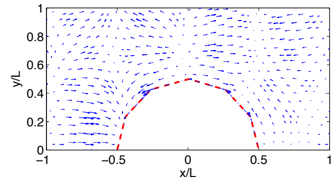
This is essential to fully benefit for complex problems

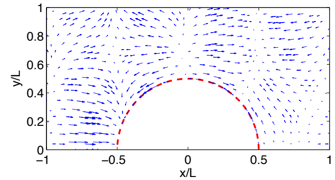
Example - Boussinesq equations

The correct representation of the boundary is essential for accuracy and speed









Example - Spherical Shallow Water equ

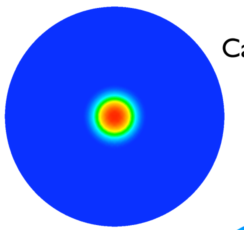
Dynamics of a thin layer of fluids on a sphere

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

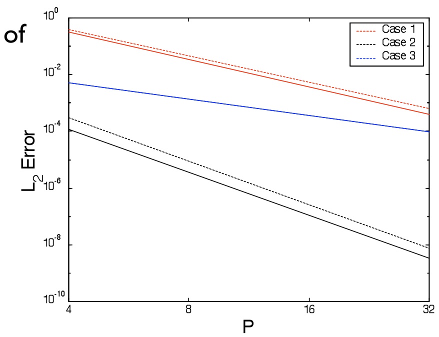
$$\frac{\partial\overline{\varphi}}{\partial t}+\nabla\cdot\overline{F}=S(\overline{\varphi})$$

Stardard benchmark (Williamsson) in geophysical flow modeling

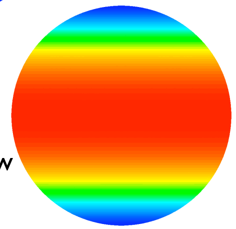
Example - Spherical Shallow Water equ



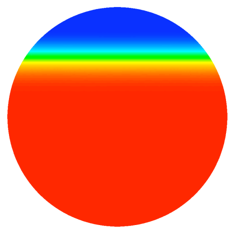
Case I: Rotation of cosine wave



Case II: Zonal Geostrophic Flow



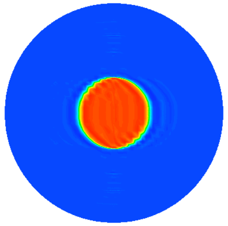
Case III: Zonal flow w/ compact support



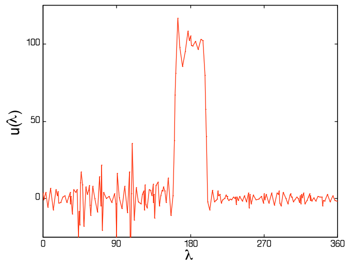
Example - Spherical Shallow Water equ

Rotation of cylinder

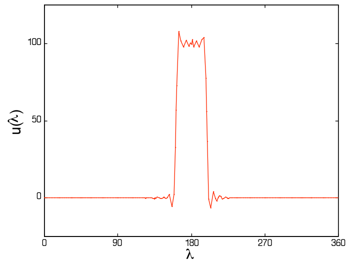
N=8



SEM



DG-FEM



An easy path to curvilinear elements

There are several good reasons for adding the support for curvilinear elements

This is work by Prof T. Warburton

✓ Higher accuracy

✓ Resolution set by solution, not geometry

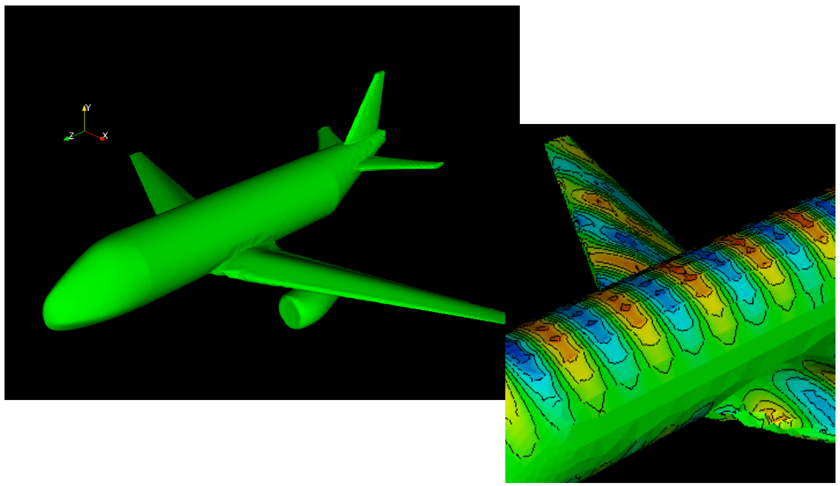
✓ Often essential to make high-order competitive

.. but classic/general approach is expensive in work and memory due to local operators

We present a special approach for linear problems

Classic curvilinear elements

Ignoring the problem is not a good idea



Another way

The idea is to define

$$\mathbf{H} = \frac{\tilde{\mathbf{H}}}{\sqrt{J}}, \mathbf{E} = \frac{\tilde{\mathbf{E}}}{\sqrt{J}}$$

and the corresponding test function

$$L_j(\mathbf{x}) = \frac{L_j(\mathbf{x})}{\sqrt{J}}$$

These are non-polynomial functions

$$\int_D H L_j \, d\mathbf{x} = \int_D J^{-1} \tilde{H} \tilde{L}_j \, d\mathbf{x} = \int_I \tilde{H} \tilde{L}_j \, d\mathbf{r}$$

Mass matrix is unchanged

Another way

The scheme becomes

$$0=\left(\tilde{\phi},\frac{\partial \mu \tilde{H}}{\partial t}\right)_{\hat{T}}+\left(\tilde{\phi},\nabla\times\tilde{E}\right)_{\hat{T}}+\left(\frac{\tilde{\phi}}{\sqrt{J}},n\times\left(E^{*}-E\right)\right)_{\partial T}-\left(\tilde{\phi},\frac{\nabla J}{2J}\times\tilde{E}\right)_{\hat{T}}$$

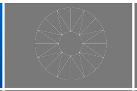
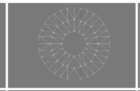
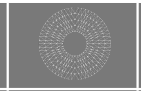
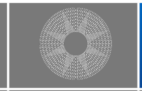
$$0=\underbrace{\left(\tilde{\psi},\frac{\partial \varepsilon \tilde{E}}{\partial t}\right)_{\hat{T}}-\left(\nabla\times\tilde{\psi},\tilde{H}\right)_{\hat{T}}}_{\text{Maxwell's equations on reference element}}\underbrace{-\left(\frac{\tilde{\psi}}{\sqrt{J}},n\times H^{*}\right)_{\partial T}}_{\text{Distributional derivative contribution}}\underbrace{+\left(\tilde{\psi},\frac{\nabla J}{2J}\times\tilde{H}\right)_{\hat{T}}}_{\text{Transform terms}}$$

Stability can still be established by standard means

This is a low-storage curvilinear formulation

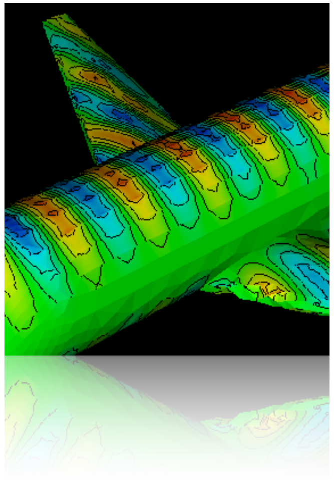
.. only for linear problems

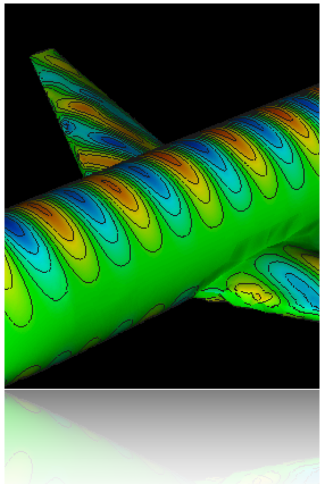
Another way

Method	N					Est. Order
DGTD	5	2.45E-04	8.06E-06	2.56E-05	5.24E-09	5.61
	6	4.31E-05	1.43E-06	2.52E-08	2.81E-10	6.49
Low storage	5	2.44E-04	8.03E-06	2.55E-05	5.22E-09	5.61
	6	4.29E-05	1.43E-06	2.52E-08	2.79E-10	6.50

No loss in accuracy

Another way





Summary of Part I

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 !

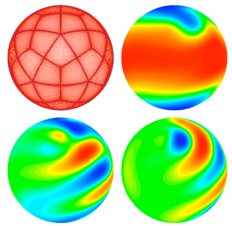
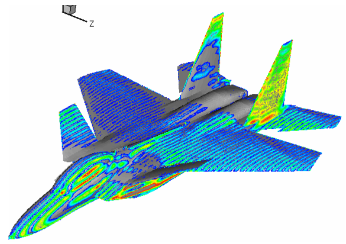
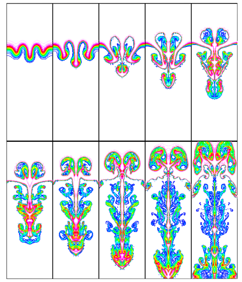
Lecture 8

- ✓ 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

The need for speed !

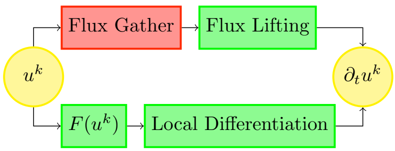
So far, we have focused on 'simple' serial computing using Matlab based model.

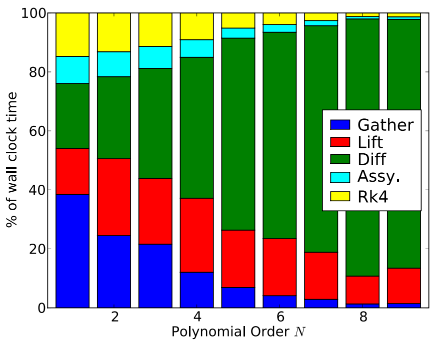
However, this will not suffice for many applications

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
- ✓ A similar line of arguments can be used for iterative solvers.

Parallel performance

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

High performance is achieved through -

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

Challenges -

- ✓ Efficient parallel preconditioning

Parallel computing

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 50Tflop/s performance.

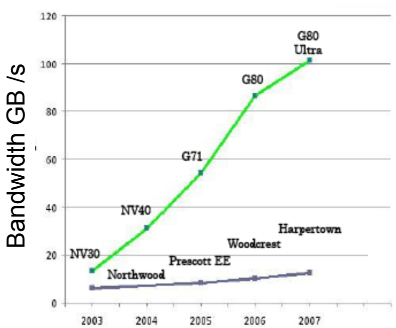
What we need is supercomputing on the desktop

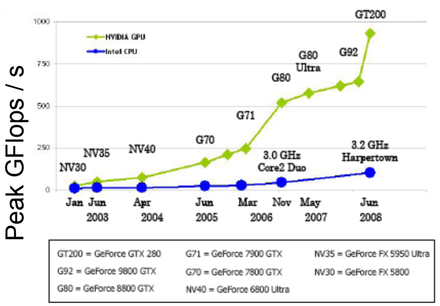
For FREE !

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

CPUs vs GPUs

Notice the following





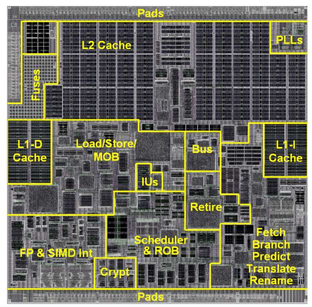
The memory bandwidth and the peak performance on Graphics cards (GPU's) is developing MUCH faster than on CPU's

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

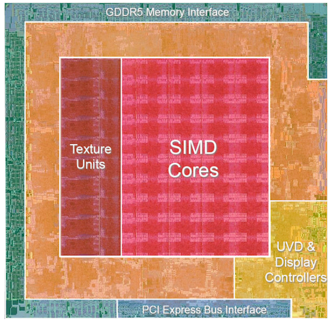


Lots of very complex logic to predict behavior

But why is this ?

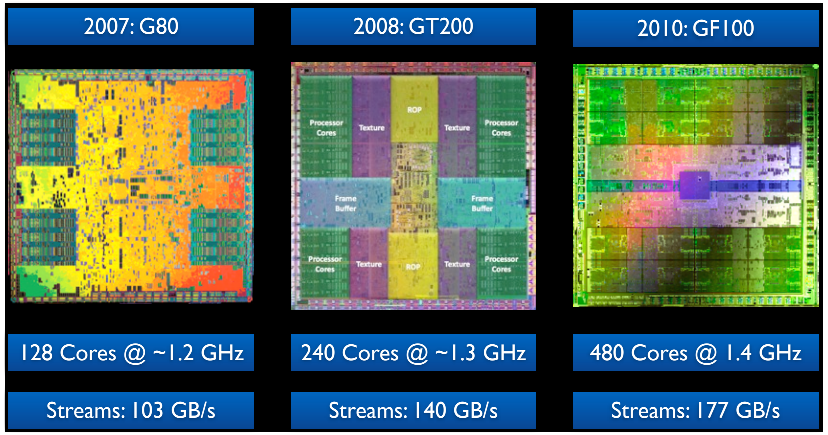
For streaming/graphics cards it is different

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



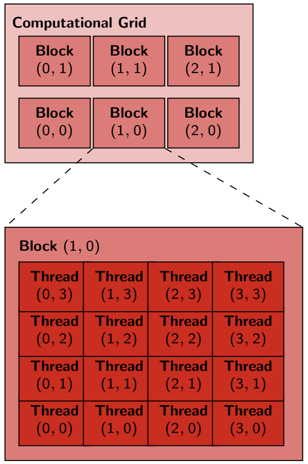
Much simpler logic with a focus on performance

But why is this ?



Core numbers grow faster than bandwidth

GPUs 101

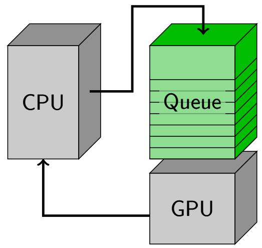


- ✓ Genuine multi-tiered parallelism
  - ✓ Grids
  - ✓ blocks
  - ✓ threads
- ✓ Only threads within a block can talk
  - ✓ Blocks must be executed in order
- ✓ Grids/blocks/threads replace loops
- ✓ Until recently, only single precision
- ✓ Code-able with CUDA (C-extension)

CPUs vs GPUs

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

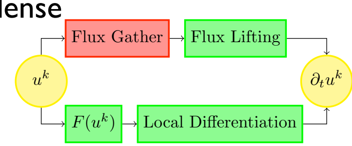
Nodal DG on GPU's

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

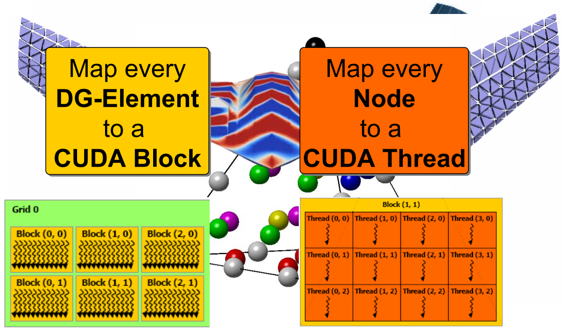
✓ GPU global memory favors dense data
➡ Local DG operators are all dense



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

Nodal DG on GPU's

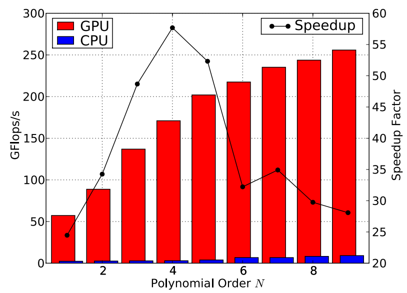
Nodes in threads, elements for blocks



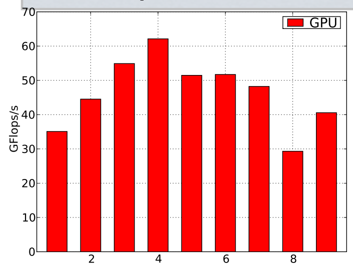
Other choices:
✓D-matrix in shared, data in global (small N)
✓Data in shared, D-matrix is global (large N)

Computing without the CPU

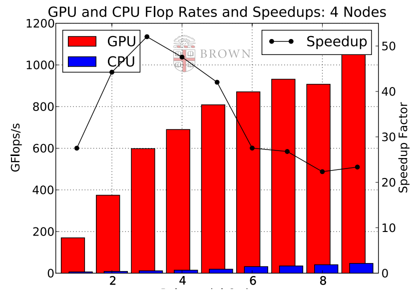
DG-FEM on one GPU



Where you need it most

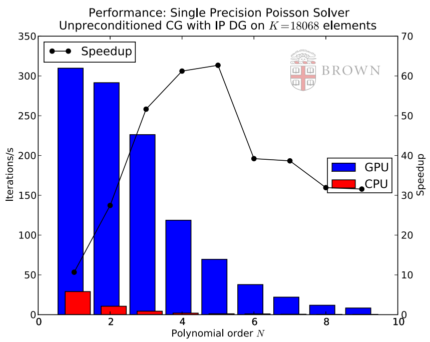


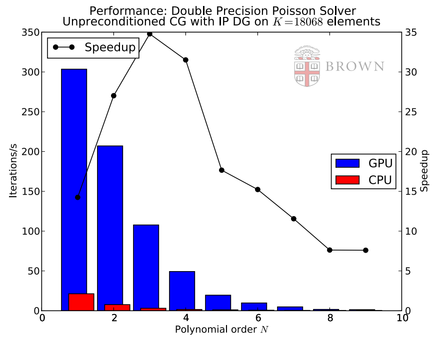
DG-FEM on four GPU one card



Nodal DG on GPU's

Similar results for DG-FEM Poisson solver with CG

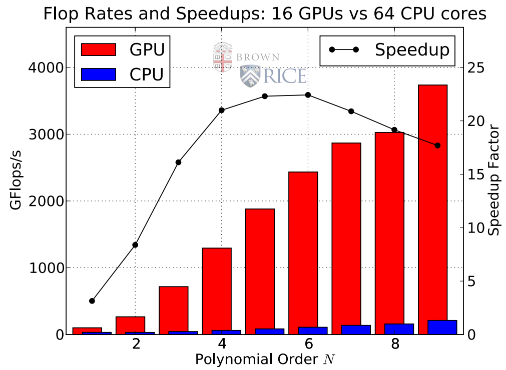


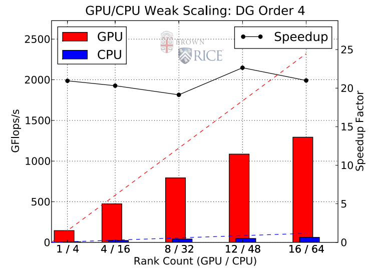


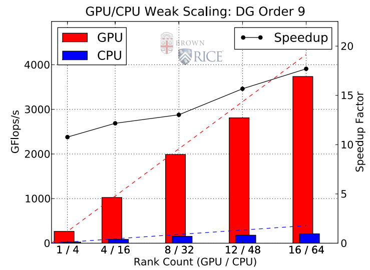
Note: No preconditioning

Combined GPU/MPI solution

MPI across network

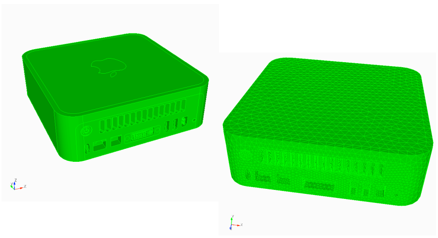


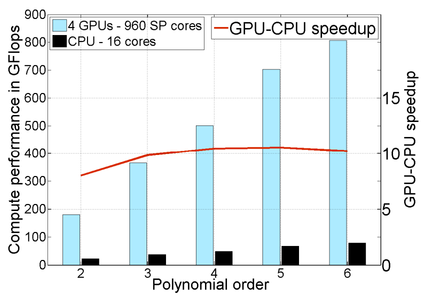


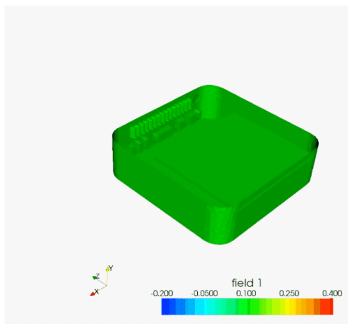


Good scaling when problem is large

Example - a Mac Mini



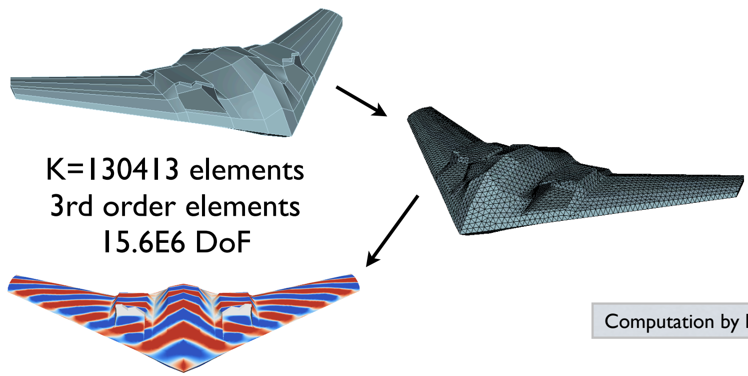




K=201765 elements
3rd order elements

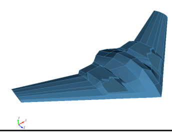
Computation by N. Godel

Example: Military aircraft



K=130413 elements
3rd order elements
15.6E6 DoF

Computation by N. Godel

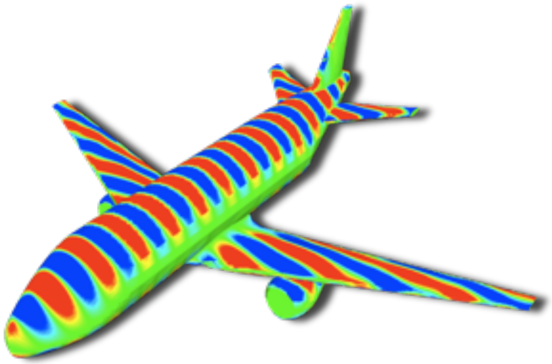
	CPU global	29 h 6 min 46 s	1.0
	GPU global	39 min 1 s	44.8
	GPU multirate	11 min 50 s	147.6

Nodal DG on GPU's

Not just for toy problems

228K elements
5th order elements
78m DOF
68k time-steps

Time ~ 6 hours

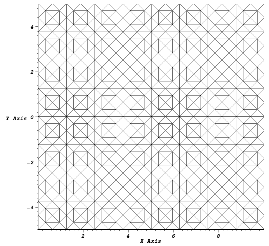


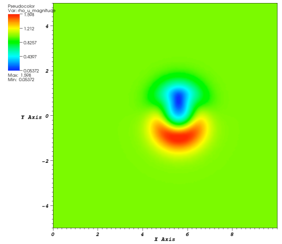
711.9 GFlop/s on one card

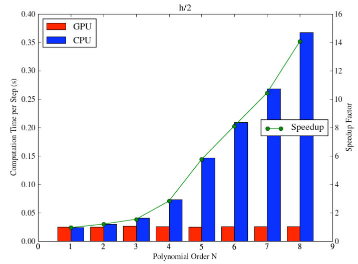
Computation by N. Godel

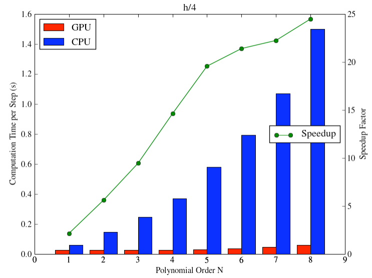
Beyond Maxwell's equations

2D Euler test case



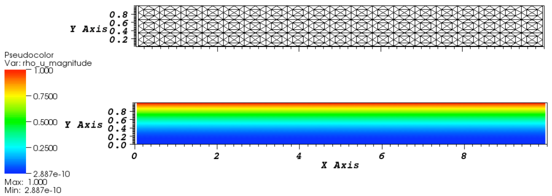


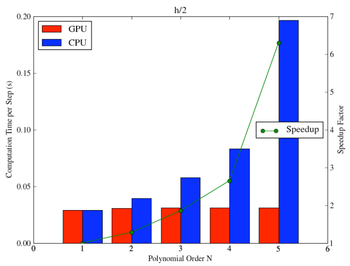


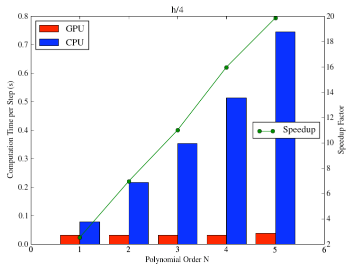


Beyond Maxwell's equations

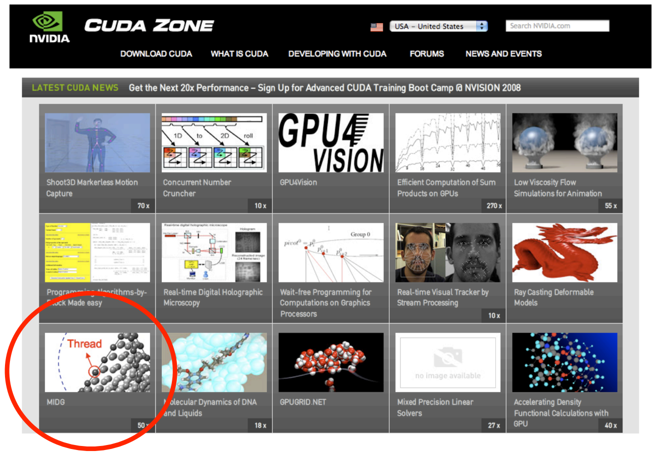
2D Navier-Stokes test case







Want to play yourself ?



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

Nodal DG on GPU's

Several GPU cards can be coupled over MPI at minimal overhead (demonstrated). Lets do the numbers

One 1TF/s/4GB mem card costs ~$8k

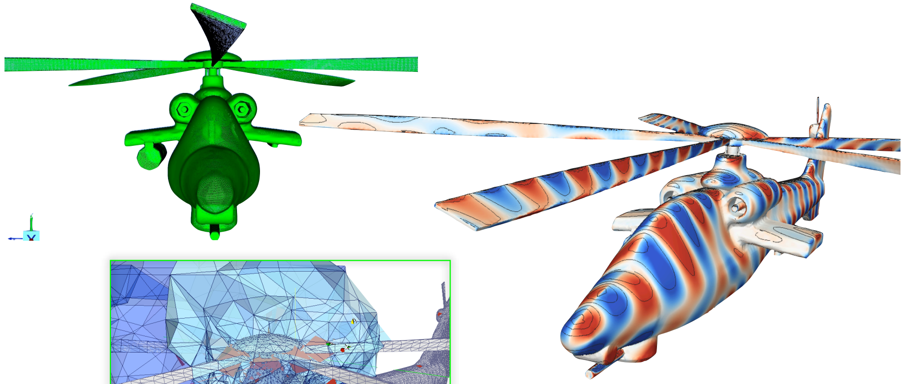
So $250k will buy you 40TFlop/s sustained

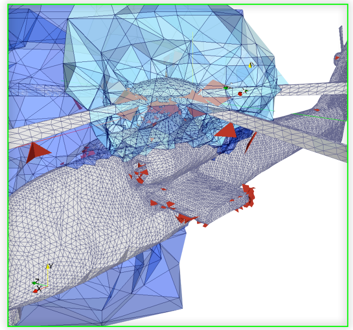
This is the entry into Top500 Supercomputer list !

... at 5%-10% of a CPU based machine

This is **a game changer** -- and the local nature of DG-FEM makes it very well suited to take advantage of this

Combining all the pieces





By T. Warburton

Do we have to write it all ?

No :-)

✓ Book related codes - all at www.nudg.org

✓ Matlab codes

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

✓ hedge - a Python based meta-programming code. Support for serial/parallel/GPU

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

Do we have to write it all ?

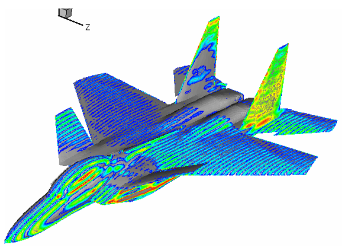
Other codes

✓ **Slegde++** - C++ operator code. Interfaced with parallel solvers (Trilinos and Mumps) and support for adaptivity and non-conformity. Contact Lucas Wilcox (NPS Monterey)

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

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

Progress ?



Year 2001

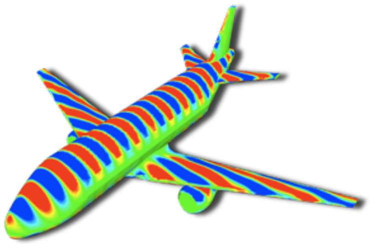
250k tets, 4th order
50m dof,100k timesteps

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 (NPS Monterey)
- ✓ Andreas Kloeckner (NYU/Courant)
- ✓ Nico Goedel (Hamburg)
- ✓ Hendrick Riedmann (Stuttgart)
- ✓ Francis Giraldo (NPS Monterrey)
- ✓ Per-Olof Persson (UC Berkeley)

... and to you for hanging in there !