Modeling Continuum PDEs using the Discontinuous Galerkin Method with OpenACC

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Scalable **A**lgorithms **a**nd **N**umerical Methods **i**n **C**omputing **(SATANIC)** Lab
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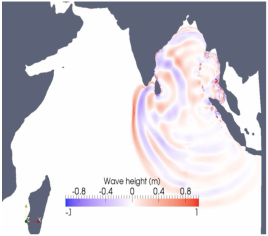
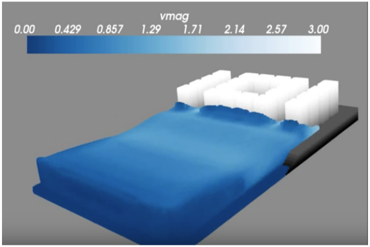
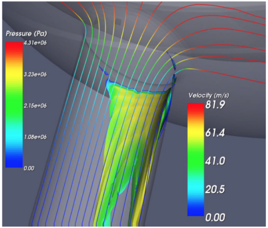
Motivation: Complex Large Scale Simulations



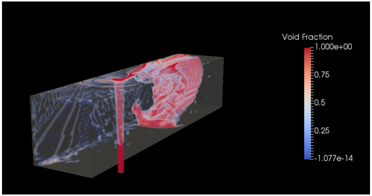
Tsunami Modeling



Coastal Inundation from Storm surges and Tsunamis



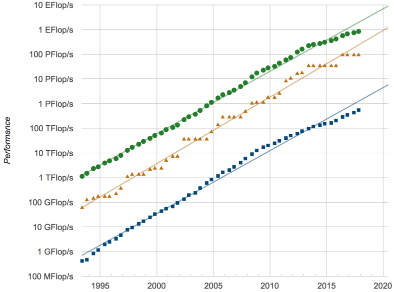
Non–equilibrium flows in Injectors



Jets in crossflows

March towards Exascale

- Growth in supercomputing performance

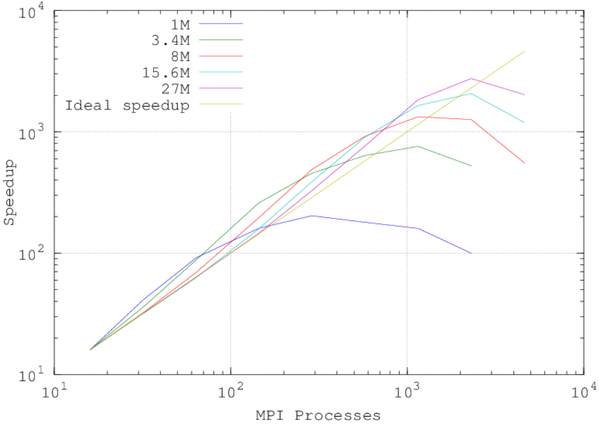


credit: top500.org

- Are current numerical methods scalable?
- Are current numerical methods power efficient?

Parallel Scaling of Finite Volume Methods

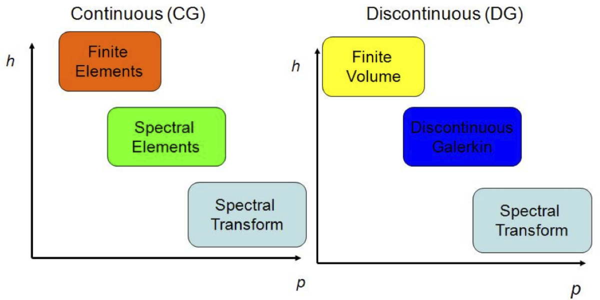
Lid driven cavity: Incompressible flow solver using OpenFOAM (Opensource FVM).



credit: hpc.ntnu.no

Element Based Galerkin methods

- All EBG methods partition the domain into computational elements and then approximate a function via basis functions.
- Examples: Finite Element, Spectral Elements, Finite Volume, Discontinuous Galerkin.



Solution Vector Approximation

- For the canonical equation

$$\frac{\partial q}{\partial t} + \frac{\partial f}{\partial x} = 0$$

  where $q = q(x,t)$, $f = f(x,t)$ and $f = qu$.

- We approximate the solution variable as

$$q_N(x,t) = \sum_{i=0}^{N} \psi_i(x) q_i(t)$$

  where $f_N = f(q_N(x,t))$.

- q being the expansion coefficients, ψ the basis functions and the N the order of the polynomial.

Differential to Integral form

- Substituting the approximation into the PDE yields

$$\frac{\partial q_N}{\partial t} + \frac{\partial f_N}{\partial x} = r \neq 0$$

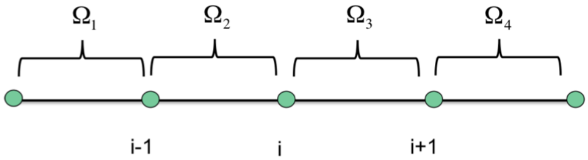
  Since we have used a finite dimensional approximation.

- We resolve this by multiplying the approximation with a test function ψ and integrating to get

$$\int_{\Omega_e} \psi_i \frac{\partial q_N}{\partial t} d\Omega_e + \int_{\Omega_e} \psi_i \frac{\partial f_N}{\partial x} d\Omega_e = \int_{\Omega_e} \psi_i r d\Omega_e \equiv 0$$

Differential to Integral form

- where the domain is partitioned as



where $\Omega = \bigcup_{e=1}^{N_e} \Omega_e$ defines the total domain and $e = 1, 2, \ldots, N_e$ are the elements

Weak Integral form

- Using calculus identities we can simplify the weak integral system into the form

$$\int_{\Omega_e} \psi_i \frac{\partial q_N}{\partial t} d\Omega_e + \int_{\Omega_e} (\psi_i f_N) d\Omega_e - \int_{\Omega_e} \frac{\partial \psi_i}{\partial x} f_N d\Omega_e = 0$$

Integrating the second term gives:

$$\int_{\Omega_e} \psi_i \frac{\partial q_N}{\partial t} d\Omega_e + [\psi_i f_N]_{\Gamma_e} - \int_{\Omega_e} \frac{\partial \psi_i}{\partial x} f_N d\Omega_e = 0$$

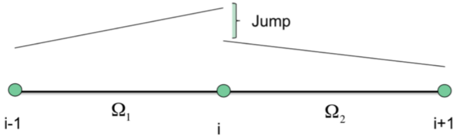
where the term in the square brackets is evaluated at the boundary Γ_e of the element Ω_e.

Discontinuous Galerkin Method

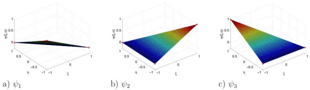
- The equation

$$\int_{\Omega_e} \psi_i \frac{\partial q_N}{\partial t} d\Omega_e + [\psi_i f_N]_{\Gamma_e} - \int_{\Omega_e} \frac{\partial \psi_i}{\partial x} f_N d\Omega_e = 0$$

  represents the (weak) integral form of the original differential equation.
- The term $[\psi_i f_n]_{\Gamma_e}$ allows neighbouring elements to communicate.

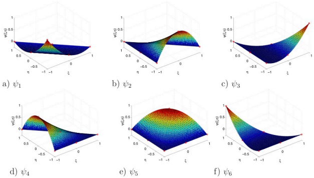


Basis functions



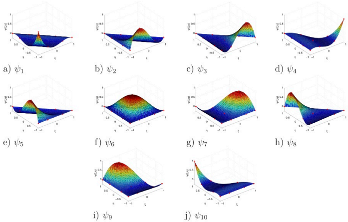
a) ψ_1 b) ψ_2 c) ψ_3

N=1



a) ψ_1 b) ψ_2 c) ψ_3 d) ψ_4 e) ψ_5 f) ψ_6

N=2



a) ψ_1 b) ψ_2 c) ψ_3 d) ψ_4 e) ψ_5 f) ψ_6 g) ψ_7 h) ψ_8 i) ψ_9 j) ψ_{10}

N=3

Discontinuous Galerkin Method

Applying DG to the Constitutive equations to obtain the weak form

$$\int_{\Omega_e} \left(\frac{\partial q_N^{(e)}}{\partial t} - F_N^{(e)} \cdot \nabla - S_N^{(e)} \right) \psi_i(x)\, dx = -\sum_{l=1}^{3} \int_{\Gamma_e} \psi_i(x)\, n^{(e,l)} \cdot F_N^{(*,l)} dx$$

Rusanov Numerical Flux

$$F_N^{(*,l)} = \frac{1}{2} \left[F_N\left(q_N^{(e)}\right) + F_N\left(q_N^{(l)}\right) - |\lambda^{(l)}| \left(q_N^{(l)} - q_N^{(e)}\right) n^{(e,l)} \right]$$

Matrix form of semi−discrete equations

Using the polynomial approximation $q_N = \sum_{i=1}^{M_N} \psi_i q_i$

$$\int_{\Omega_e} \psi_i \psi_j dx \frac{\partial q^{(e)}}{\partial t} - F_j^{(e)} \cdot \int_{\Omega_e} \nabla \psi_i \psi_j dx - \int_{\Omega_e} \psi_i \psi_j dx S_j^{(e)} = - \sum_{l=1}^{3} \int_{\Gamma_e} \psi_i \psi_j n^{(e,l)} dx \cdot (F^{(*,l)})_j$$

Defining element matrices as

$$M_{ij}^{(e)} = \int_{\Omega_e} \psi_i \psi_j dx, \quad M_{ij}^{(e,l)} = \int_{\Gamma_e} \psi_i \psi_j n^{(e,l)} dx, \quad D_{ij}^{(e)} = \int_{\Omega_e} \nabla \psi_i \psi_j dx$$

Matrix form of semi−discrete equations

$$M_{ij}^{(e)}\frac{\partial q^{(e)}}{\partial t} - (D_{ij}^{(e)})^{\mathcal{T}} F_j^{(e)} - M_{ij}^{(e)} S_j^{(e)} = -\sum_{l=1}^{3} (M_{ij}^{(e,l)})^{\mathcal{T}} (F^{(*,l)})_j$$

Eliminating mass matrix on LHS

$$\widehat{D}^{(e)} = (M^{(e)})^{-1} D^{(e)}, \quad \widehat{M}^{(e,l)} = (M^{(e,l)})^{-1} M^{(e,l)}$$

$$\frac{\partial q^{(e)}}{\partial t} - (\widehat{D_{ij}}^{(e)})^{\mathcal{T}} F_j^{(e)} - S_j^{(e)} = -\sum_{l=1}^{3} (\widehat{M}_{ij}^{(e,l)})^{\mathcal{T}} (F^{(*,l)})_j$$

Matrix form of semi−discrete equations

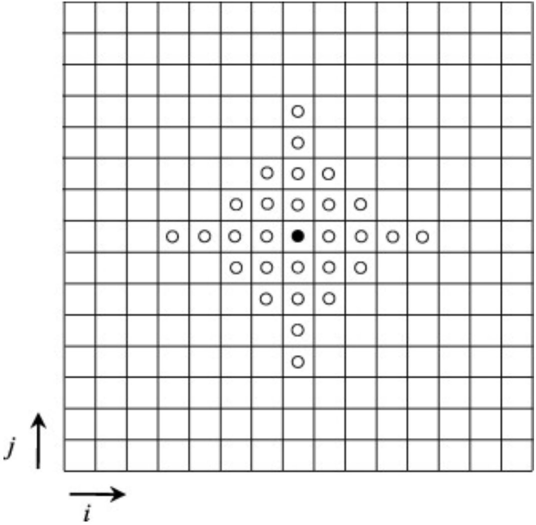
$$M_{ij}^{(e)}\frac{\partial q^{(e)}}{\partial t} - \underbrace{(D_{ij}^{(e)})^{\mathcal{T}} F_j^{(e)} - M_{ij}^{(e)} S_j^{(e)}}_{\text{Volume Integration (offload)}} = \underbrace{-\sum_{l=1}^{3}(M_{ij}^{(e,l)})^{\mathcal{T}}(F^{(*,l)})_j}_{\text{Flux Integration (offload)}}$$

Eliminating mass matrix on LHS

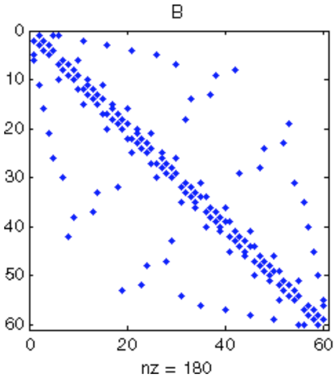
$$\widehat{D}^{(e)} = (M^{(e)})^{-1} D^{(e)}, \quad \widehat{M}^{(e,l)} = (M^{(e,l)})^{-1} M^{(e,l)}$$

$$\frac{\partial q^{(e)}}{\partial t} - (\widehat{D_{ij}}^{(e)})^{\mathcal{T}} F_j^{(e)} - S_j^{(e)} = -\sum_{l=1}^{3}(\widehat{M}_{ij}^{(e,l)})^{\mathcal{T}}(F^{(*,l)})_j$$

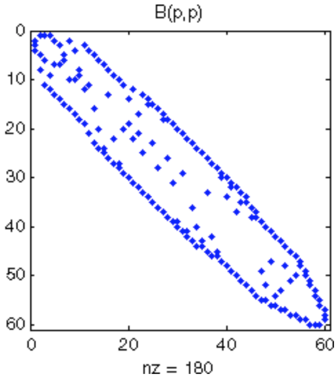
Finite volume Stencil



Sparsity Pattern: Finite volume



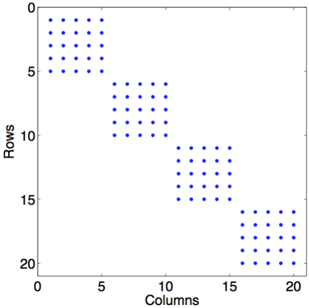
Unordered Matrix



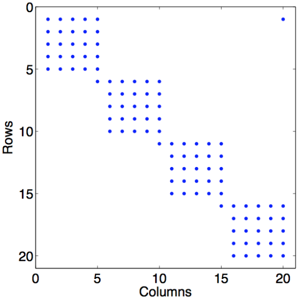
Ordered Matrix RCM

Credit:Mathworks.com

Sparsity Pattern: Discontinuous Galerkin

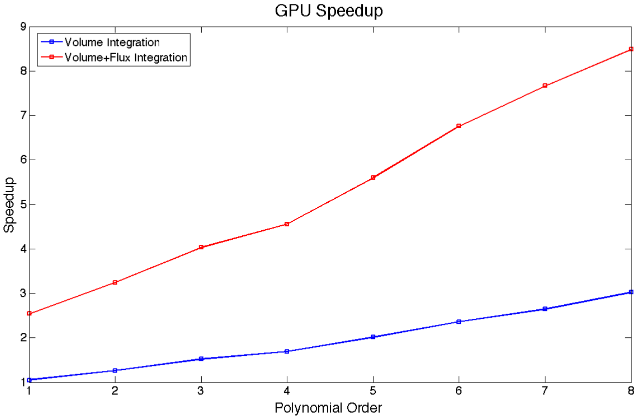


Mass Matrix

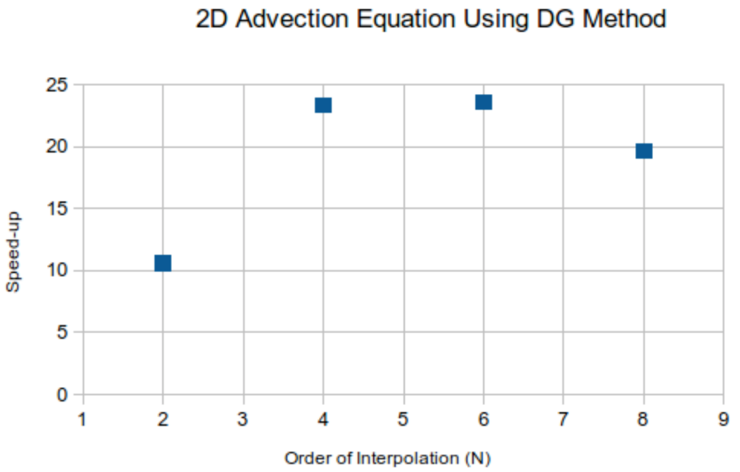


Differentiation Matrix

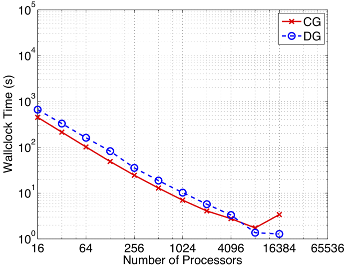
Speedup on GPUs



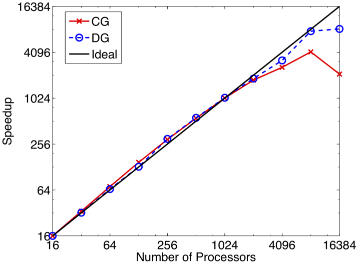
Speedup on GPUs: Optimised for N=4



Scaling: Discontinuous Galerkin with N=4



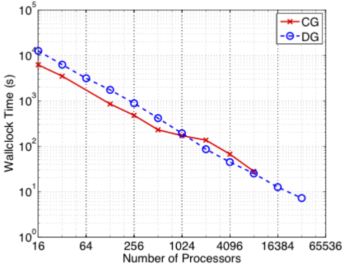
(a) wallclock time



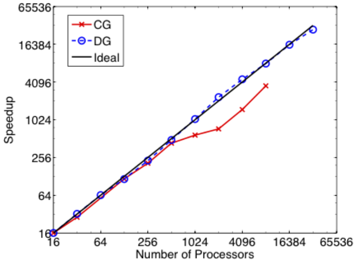
(b) speedup

Girlado et al, Continuous and discontinuous Galerkin methods for a scalable three-dimensional nonhydrostatic atmospheric model: Limited-area mode, JCP (2012)

Scaling: Discontinuous Galerkin with N=8



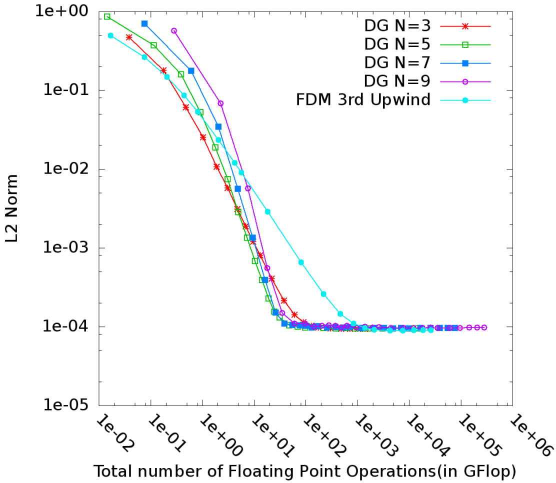
(a) wallclock time



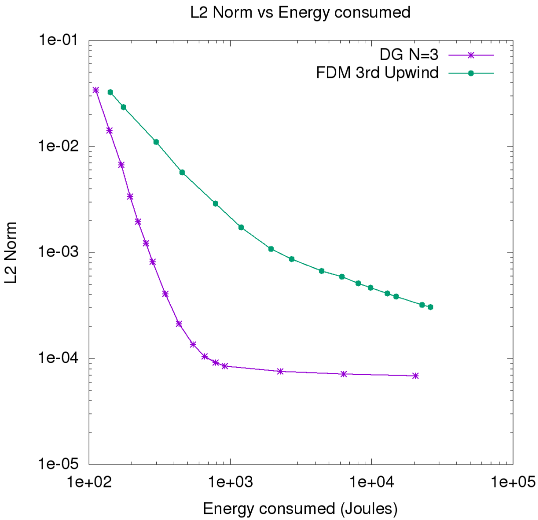
(b) speedup

Girlado et al, Continuous and discontinuous Galerkin methods for a scalable three-dimensional nonhydrostatic atmospheric model: Limited-area mode, JCP (2012)

Error vs Computational Efficiency



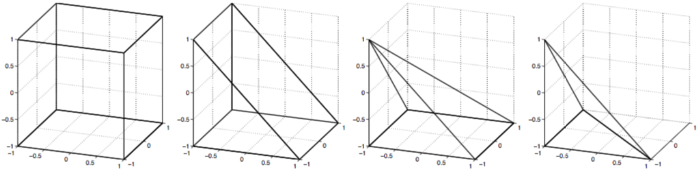
Power Efficiency



MEANDG Framework

- C++ based framework.
- Fully three dimensional. Support for Hexahedral, Tetrahedral and transitional prism, pyramid cells.
- Complete abstraction. Discrete operators can work with Scalar, Vector and Tensor objects.
- Can quickly develop solvers based on Continuum PDEs.
- Currently solver for Advection, Euler and Navier–Stokes Equations are present.
- Parallel implementation using OpenMP, OpenACC and MPI.

Geometry Support

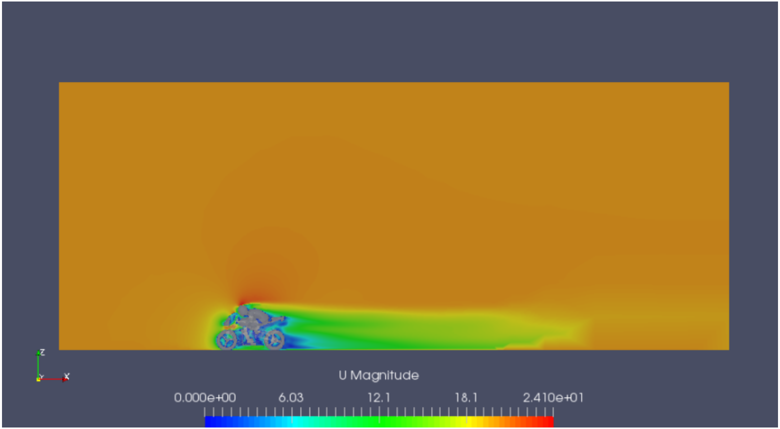


(a) Hexahedra (b) Prism (c) Tetrahedra (d) Pyramid

- Higher order support through cardinal Lagrange polynomials.
- Polynomials upto 16th order have been tested.
- Natural support for h and p refinement.

Complex Geometry

- Flow past a motorbike.



Three dimensional Westervelt Equations

- Discontinuous Galerkin code based on the Westervelt equation to simulate transient acoustic wave propagation in the brain and skull.
- Collaborators : James F. Kelly, Michigan State University and Simone Marras, Rutgers University
- Ongoing, only 12 routines have been parallelized via OpenACC.
- Speedup: 4.62
- GPU used: Nvidia V100 (PSG Cluster)

GPU Bootcamp at IIT Bombay

- 13 research groups with approximately 30 researchers and 6 mentors. Held May 7th and 8th 2019
- Application domains
  - Computational Fluid Dynamics
  - Materials Science
  - Physics
  - Computational Biology
  - Earth systems.
- Groups had either serial code or MPI parallel code.
- With OpenACC the max speedup achieved by a group was 40x. most groups reported some amount of speedup.

Conclusions

- To solve complex problems we need more detailed simulation capability which in turn requires more than ever computational power.
- Current numerical methods technology has limits on issues of scaling.
- Newer methods are required. DG promises to show linear scaling up to thousands, if not hundreds of thousands of processors.
- Power efficiency is desired and DG demonstrates power savings to large extent.
- Numerical methods have to adapt to newer computational hardware rather than vice versa.