Development of Spectral Element Methods for Compressible Flow Problems

David A. Kopriva

Department of Mathematics
The Florida State University
Spectral Multidomain Methods

1980’s
- Limited
- Inflexible
- Complicated

Today
- Powerful
- Robust
- Flexible

Fig. 10. Multidomain grid with six subdomains for the Ringleb problem.
1983: Flow Over a Cylinder

- Problem (Hussaini):
  
  *Find, precisely, the transonic Mach number for a cylinder*

- Approach:
  - Chebyshev spectral method
  - Euler Gas-Dynamics equations

(Contour Plot: Hafez & Wahba, 2004)
Chebyshev Spectral Collocation
Origin of Spectral Multidomain
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Timeline

- 1980’s: Baby Steps
  - Strong form Chebyshev collocation

- 1990’s: Search for the Ultimate Scheme™
  - Cell Average FCT (Karniadakis)
  - Penalty method (Hesthaven, Gottlieb, Funaro)
  - Staggered Grid (Kopriva)


- 2010s+: Large scale applications
Strong Form Chebyshev

Features:
- Standard Chebyshev Collocation in interiors
- (Characteristic) Patching conditions at interfaces

Pros:
- Lower cost per DOF than single domain
- Spectral accuracy

Cons:
- Mesh required continuous metrics
- Complicated to implement
- Not robust
90’s: Weak Imposition of BCs

Weak imposition gives full unstructured mesh flexibility.

- **Spectral Penalty method (Hesthaven)**
  - (+) Natural imposition of conditions for advection-diffusion operators
  - (+) Stability proof for linearized compressible Navier-Stokes
  - (−) Penalty parameter
  - (−) Stiff
  - (−) Not Conservative
  - (−) Ad-Hoc treatment at corners and when advection speed vanishes

- **Staggered Grid Method (Kopriva)**
  - (+) Conservative
  - (+) Easy to implement
  - (+) No special corner point operations
  - (+) Robust
  - (−) Weak instability for periodic advection problems
Staggered Grid Approximation

- Solution and fluxes in different polynomial spaces
  
  \[ Q \in P^N \times P^N \]
  
  \[ F \in P^{N+1} \times P^N \]
  
  \[ G \in P^N \times P^{N+1} \]

- Only fluxes on boundaries
- Uses Riemann solvers on discontinuous solutions
00’s : DG Spectral Element Method (DGSEM)

DGSEM:
- Conservative
- Easy BCs
- Variational Formulation
- Broad Framework

Why DG over staggered grid?
- Faster: 20% faster (Simpler Interpolations)
- More Accurate: $10\times$ on test problem
DGSEM Framework: Conservation Laws

Problems modeled by a system of conservation laws:

\[ \vec{q}_t + \nabla \cdot \vec{f} = 0 \]

\[ \vec{f} = \vec{f}^i + \vec{f}^v \]

Examples:

- **Euler Equations**

  \[ \vec{q} = \begin{bmatrix} \rho \\
  \rho \vec{u} \\
  \rho E \end{bmatrix}, \quad \vec{f}^i = \begin{bmatrix} \rho \vec{u} \\
  \rho \vec{u} \otimes \vec{u} + pI \\
  \rho uH \end{bmatrix}, \quad \vec{f}^v = 0 \]

- **Navier-Stokes Equations**

  \[ \vec{f}^v = \begin{bmatrix} 0 \\
  \tau \cdot \vec{u} + k \nabla T \end{bmatrix} \]
Multi-Element Decomposition

Subdivide domain into multiple elements
Multi-Element Decomposition

Decomposition:

- Arbitrarily complex
- Conforming or nonconforming
- Moving or stationary
Multi-Element Decomposition: 3D

(Courtesy of G. Gassner)
Mapping to Reference Element

Transform:

\[ x = X (\vec{\xi}, \tau) \]
Strong form of conservation law:

\[ \tilde{q}_t + \nabla \cdot \tilde{f} = 0 \]

where

\[ \tilde{q} = Jq \]

\[ \tilde{f}^i = J a^i \cdot (f - q x_\tau) \]

Jacobian satisfies Geometric Conservation Law:

\[ J_\tau + \nabla_\xi \cdot \tilde{\Psi}(J) = 0, \]
The DG Spectral Element Framework

Three characteristics:

1. **Approximate**
   \[\tilde{q} \approx \tilde{Q} \in \mathbb{P}^N, \quad \tilde{f} \approx \tilde{F} \in \mathbb{P}^M \text{ on } E\]

2. **Weak form**
   \[\int_E \left( \tilde{Q}_t + \nabla \cdot \tilde{F} \right) \phi = 0\]

3. **No continuity on** \(\phi \in \mathbb{P}^N\) **between elements**
DG Formulation

Integrate by parts

\[
\int_E \tilde{Q}_t \phi d\xi + \int_{\partial E} \tilde{F} \cdot \hat{n}_\xi \phi dS - \int_E \tilde{F} \cdot \nabla \phi d\xi = 0
\]

Replace boundary fluxes with Riemann solver

\[
\int_E \tilde{Q}_t \phi d\xi + \int_{\partial E} (\tilde{F} - \tilde{F}^* \cdot \hat{n}_\xi) \phi dS - \int_E \tilde{F} \cdot \nabla \phi d\xi = 0 \quad \text{Form I}
\]

Maybe integrate by parts again

\[
\int_E \tilde{Q}_t \phi d\xi + \int_{\partial E} (\tilde{F} - \tilde{F}^* \cdot \hat{n}_\xi) \phi dS - \int_E \nabla \cdot \tilde{F} \phi d\xi = 0 \quad \text{Form II}
\]
We actually have a *framework* from which to derive methods:

1. Quad/Hex or Tri/Tet elements?
2. Nodal or modal basis?
3. What polynomials?
4. Approximate boundaries with different orders?
5. Approximate solution and fluxes with different orders?
6. Exact integrals or quadrature?
7. Inexact or exact quadrature?
8. Form I or Form II?
9. ???

Too many choices can be overwhelming.
DG Spectral Element Approximation

It’s Not That Hard!
“Classical” spectral element approximation:

1. Quadrilateral/ Hexahedral elements  
   ⇒ Efficient tensor product bases
2. Nodal basis  
   ⇒ Easy for nonlinear/variable coefficient/general complex geometry problems
3. All approximations at same polynomial order  
   ⇒ Simplifies coding
4. Legendre basis  
   ⇒ Spectral accuracy, conditioning
5. Gauss-Type quadrature
Implementation

Solution and fluxes by polynomials in (Lagrange) nodal form

\[
Q = \sum_{n=0}^{N} \sum_{m=0}^{N} Q_{n,m} \ell_n(\xi) \ell_m(\eta)
\]

\[
F = \sum_{n=0}^{N} \sum_{m=0}^{N} (F_{n,m} \hat{x} + G_{n,m}) \ell_n(\xi) \ell_m(\eta).
\]

Integrate by parts 1x

\[
\int_E \frac{\partial Q}{\partial t} \phi_{i,j} d\xi + \int_{\partial E} F^* \cdot \hat{n} \phi_{i,j} dS - \int_E F \cdot \nabla \phi_{i,j} d\xi = 0
\]

With \( \phi_{i,j} = \ell_i(\xi) \ell_j(\eta) \).
Apply Quadrature to Each Integral

Time derivative integral

\[
\int_{-1,N}^{1,N} \frac{dQ(\xi, \eta)}{dt} \ell_i(\xi) \ell_j(\eta) d\xi d\eta
\]

\[
= \sum_{k=0}^{N} \sum_{l=0}^{N} \frac{dQ(\xi_k, \eta_l)}{dt} \ell_i(\xi_k) \ell_j(\eta_l) w_k^{(\xi)} w_l^{(\eta)}
\]

\[
= \frac{dQ_{i,j}}{dt} w_i^{(\xi)} w_j^{(\eta)},
\]

etc.
Spatial Discretization

On each element we integrate

\[
\frac{dQ_{i,j}}{dt} + \left\{ \left[ \tilde{F}^*(1, \eta_j) \frac{\ell_i(1)}{w_i^{(\xi)}} - \tilde{F}^*(-1, \eta_j) \frac{\ell_i(-1)}{w_i^{(\xi)}} \right] + \sum_{k=0}^{N} \tilde{F}_{k,j} \hat{D}_{ik}(\xi) \right\} \\
+ \left\{ \left[ \tilde{G}^*(\xi_i, 1) \frac{\ell_j(1)}{w_j^{(\eta)}} - \tilde{G}^*(\xi_i, -1) \frac{\ell_j(-1)}{w_j^{(\eta)}} \right] + \sum_{k=0}^{N} \tilde{G}_{i,k} \hat{D}_{jk}(\eta) \right\} = 0
\]

Primary Work:
- Computation of fluxes \( \tilde{F}_{k,j} \) and \( \tilde{G}_{i,k} \) from solution
- Computation of Riemann solver \( \tilde{F}^*(\pm 1, \eta_j) \) and \( \tilde{G}^*(\xi_i, \pm 1) \)
- Series of dot products (Gauss)
- Series of Matrix-Vector products
DGSEM Time Derivative Algorithm

Gauss-Lobatto Version:

<table>
<thead>
<tr>
<th>Equation</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\dot{Q}_j = -F'$</td>
<td>Time derivative of $Q_j$</td>
</tr>
<tr>
<td>$\dot{Q}<em>{0,j} = \dot{Q}</em>{0,j} - b_j \cdot RiemannSolver(Q_{j}^{ext}, Q_{0,j}, \hat{n}_j^L)$</td>
<td>Time derivative of $Q_{0,j}$</td>
</tr>
<tr>
<td>$\dot{Q}<em>{N,j} = \dot{Q}</em>{N,j} - b_j \cdot RiemannSolver(Q_{N,j}, Q_{j}^{ext}, \hat{n}_j^R)$</td>
<td>Time derivative of $Q_{N,j}$</td>
</tr>
</tbody>
</table>

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<tr>
<td>$\dot{Q}_i = \dot{Q}_i - G'$</td>
<td>Time derivative of $Q_i$</td>
</tr>
<tr>
<td>$\dot{Q}<em>{i,0} = \dot{Q}</em>{i,0} - b_i \cdot RiemannSolver(Q_{i}^{ext}, Q_{i,0}, \hat{n}_i^B)$</td>
<td>Time derivative of $Q_{i,0}$</td>
</tr>
<tr>
<td>$\dot{Q}<em>{i,M} = \dot{Q}</em>{i,M} - b_i \cdot RiemannSolver(Q_{i,M}, Q_{i}^{ext}, \hat{n}_i^T)$</td>
<td>Time derivative of $Q_{i,M}$</td>
</tr>
</tbody>
</table>
DG-Spectral Element Approximation

See... It’s Not That Bad!

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The Past: The Origin of Spectral Multidomain

The Present: DG Spectral Element Framework

The Future

See... It’s Not That Bad!
What We Know

- Form I and Form II are algebraically identical
- Gauss has better Phase/Dissipation properties
- Gauss-Lobatto can take larger time steps
- Gauss is more robust
- Gauss is slightly more efficient than Gauss-Lobatto
- Mesh can be moved Free-Stream Preserving with spectral and full time accuracy
- Suitable for massive parallelization
- Can be used for industrial strength™ applications
Integrate By Parts 1X or 2X?

**Theorem**

*(Kopriva and Gassner, 2010)* For quadrilateral/hexahedral tensor product discontinuous Galerkin approximations to systems of hyperbolic conservation laws with either Gauss or Gauss-Lobatto quadratures the two forms are algebraically equivalent as long as one uses global polynomial representations for the flux and solutions.
The Future
Spectral Element
Multidomain
Origin of Spectral
The Past: The
David A. Kopriva
Development of
Flow Problems
Compressible
to
sided interpolations are used to construct the rows of the derivative matrix
due to the nonuniform node distribution, the bias still stems from the fact that one-
approximations. Although no direct comparison to existing FD formulae can be made


where

8

10

N=1

N=10

N
K
*
Re(Ω
*
)
0 0.7854 1.5708 2.3562 ... n da p p l yam o d a l
filter where all filter coefficients are equal to 1 except for the last one

Fig. 4.3

Fig. 4.1

Fig. 4.2

GREGOR GASSNER AND DAVID A. KOPRIVA
N=1

N=10

N
K
*
Re(Ω
*
)
0 0.7854 1.5708 2.3562 3.1 ... and the nodal DG scheme

[13] are exact, in the sense that all integrals are evaluated exactly. Figure 4.1(a) shows
Real part of the physical mode for the Gauss–Lobatto DGSEM scheme with

Real part of the physical mode for DGSEM with

Real part of the physical mode for the Gauss DGSEM scheme with

The Gauss–Lobatto underintegration is the reduced maxima of the dispersion relation

The same analysis for the DGSEM with Gauss–Lobatto nodes reveals a signifi-
cantly different behavior between the two schemes. The results of this analysis are
presented in Figure 4.3, where again the dispersion relation and the logarithm of the
curves and thus a drastic reduction of the overshoots. Up to about degree


The Discrete Physical Mode

The Discrete Physical Mode

The Discrete Physical Mode

(a) Dispersion relation

(b) Logarithm of dispersion error

(a) Dispersion relation

(b) Logarithm of dispersion error

Gauss Has Better Dispersion Error
Gauss Has Better Dissipation Error

Fig. 6.1. Imaginary part of the physical mode for the Gauss DGSEM scheme with \(N = 1\) up to \(N = 10\). In the logarithmic plot, the error is cut off at \(10^{-10}\) to avoid numerical noise.

We note that we did not include the compact Finite Difference scheme for comparison, as this standard central differencing approach yields a dissipation error equal to zero. The additional stability and dissipation needed for the approximation of nonlinear equations within those schemes is provided by filtering techniques that are not well suited for comparison since the effect depends on the implementation, the time integration method and the time step.

Comparing the dissipation relations of the Gauss and the Gauss-Lobatto DGSEM reveal that again the Gauss scheme is the more accurate one. For a detailed quantification, we look again at the points per wavelength for a given dissipation error

\[
\delta := |\text{Im}(\Omega(K))|.
\]

The results are listed in Table 6.1 and 6.2. We can see that the advantage of the Gauss scheme decreases with increasing polynomial degree \(N\), which is similar when comparing the dispersion accuracy of both schemes. Evaluating the resolution requirements for the Gauss scheme we get the well known result that the dispersion error is dominated by the dissipation errors and that the accuracy requirements for the dissipation are more severe, Hu et al. [12]. However in the case of the Gauss-Lobatto scheme we...
Gauss is Slightly More Efficient Overall

**Figure:** Maximum error as a function of work for the Gauss and Lobatto approximations. Left: Uniform mesh. Right: Non-Uniform Mesh
Free-Stream Preservation and the Geometric Conservation Law

Theorem

(Acosta & Kopriva, 2012) Suppose that at time $\tau^n$, $Q^n_{i,j} = c$, where $\vec{c}$ is a constant vector. Define $Q_{i,j} \equiv \tilde{Q}_{i,j}/\tilde{J}_{i,j}$, where $\tilde{J}_{i,j}$ is the solution of the GCL. Then

$$Q^{n+1}_{i,j} = c.$$ 

Spectral + High order time accuracy when moving mesh by:

- **Method 1**: Exact differentiation of the mapping.
- **Method 2**: Integration of an acceleration equation.
- **Method 3**: Numerical differentiation of the mesh position via the time integrator (Inverse operator).
Example: Time Accurate Moving Mesh
Example: Time Accuracy on Moving Mesh

![Graph showing time accuracy on moving mesh](image-url)
Massive Parallelization (G. Gassner)
Industrial Strength Applications: Natural Gas Injector Acoustics

(Courtesy of G. Gassner)
Industrial Strength Applications: Natural Gas Injector Acoustics

(Courtesy of G. Gassner)
The Future: What We Still Want to Know

- How mesh affects accuracy and time step
- How to couple (moving) material interfaces
- How to move meshes efficiently
- How to solve time accurate problems efficiently
  - Implicit Schemes
  - Preconditioning
  - Local Time Stepping
- How to guarantee stability - Aliasing removal
- How to compute shocks
- Adaptation

AND …
1983 + 30: Flow Over a Cylinder

• Problem (Hussaini):

Find, precisely, the Mach number where flow over cylinder goes transonic.

(Contour Plot: Hafez & Wahba, 2004)
1983 + 30: Flow Over a Cylinder

STILL NOT DONE YET!