

#### Using High-Order Element-based Galerkin Methods to capture Hurricane Intensification

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- U.S. Navy's NEPTUNE dynamics is based on NUMA. For more info see: <u>https://frankgiraldo.wixsite.com/mysite/numa</u>
- xNUMA is a light-weight version of NUMA designed specifically for the MMF + MR work presented here. More info can be found at: <u>https://frankgiraldo.wixsite.com/mysite/xNUMA</u>



## <u>Motivation</u>

Hurricane Rapid Intensification (RI) (where max wind velocities exceed ~30 mph within 24hour period) continues to be an important topic to understand extreme weather.



- ▶ To properly capture RI requires LES models at  $\Delta x = \mathcal{O}(100 \, m)$  that run **stably** with as little **dissipation** as possible. Running a CRM at this resolution is still too expensive (cannot be done on a regular basis). Our simulations in [1] were run at  $\Delta x = \mathcal{O}(2 \, km)$  (CRM with 80 million DoF). LES would require 32 billion DoF with  $\Delta t$  20x smaller (i.e.,  $\mathcal{O}(10^4)$  more expensive).
- To run such simulations require different strategies: to resolve fine-scale features, for timeintegration, and in high-performance computing.

#### **Governing Equations**

Compressible Euler Equations (Non-hydrostatic)

$$\stackrel{\flat}{=} \frac{\partial \rho}{\partial t} + \nabla \cdot \left( \rho \mathbf{u} \right) = 0,$$

$$\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} + \frac{1}{\rho} \nabla P + \nabla \phi + \mathbf{\Omega} \times \mathbf{u} = S_P(\mathbf{u}),$$

$$\frac{\partial \theta}{\partial t} + \mathbf{u} \cdot \nabla \theta = S_P(\theta)$$

$$\stackrel{\flat}{=} \frac{\partial q_i}{\partial t} + \mathbf{u} \cdot \nabla q_i = S_P(\mathbf{q_i}), \ i = 1, \dots, M_{water}$$

NUMA also carries an internal energy form (used for space weather applications) [2] and two conservation forms (used for Entropy-Stable work).

# Element-based Galerkin Methods [3]



[3] F.X. Giraldo. An Introduction to Element-Based Galerkin Methods on Tensor-Product Bases: Analysis, Algorithms, and Applications, Springer Texts in Computational Science and Engineering, Series Volume 24, ISBN: 978-3-030-55068-4 (2020)

#### <u>Continuous/discontinuous Galerkin methods</u>

Governing equation:

$$\frac{\partial \mathbf{q}}{\partial t} + \nabla \cdot \mathbf{F}(\mathbf{q}) = S(\mathbf{q})$$

Approximate the **global** solution as:

$$q_N^{(e)}(\mathbf{x},t) = \sum_{j=1}^{M_N} \psi_j(\mathbf{x}) q_j^{(e)}(t) \qquad \begin{array}{l} \mathbf{F}_N = \mathbf{F}(\mathbf{q}_N) \\ S_N = S(\mathbf{q}_N) \end{array}$$

Define residual:

$$R\left(q_{N}^{(e)}\right) \equiv \frac{\partial \mathbf{q}_{\mathbf{N}}^{(e)}}{\partial t} + \nabla \cdot \mathbf{F}_{N}^{(e)} - S_{N}^{(e)} = \epsilon$$

#### **Problem statement:**

Find 
$$\mathbf{q}_N \in S$$
  $\forall \psi \in S$    
 $\begin{cases} \mathcal{S}_{CG} = \{\psi \in H^1(\Omega) : \psi \in P_N(\Omega_e) \ \forall \Omega_e\} \\ \mathcal{S}_{DG} = \{\psi \in L^2(\Omega) : \psi \in P_N(\Omega_e) \ \forall \Omega_e\} \end{cases}$ 
such that
$$\int_{\Omega_e} \psi_i R(\mathbf{q}_N) \mathrm{d}\Omega_e = 0$$

#### <u>Continuous/discontinuous Galerkin methods</u>

Integral form:  

$$\int_{\Omega_{e}} \psi_{i} R(\mathbf{q}_{N}^{(e)}) d\Omega_{e} = 0$$

$$\int_{\Omega_{e}} \psi_{i} \frac{\partial \mathbf{q}_{N}^{(e)}}{\partial t} d\Omega_{e} + \int_{\Omega_{e}} \psi_{i} \nabla \cdot \mathbf{F}_{N}^{(e)} d\Omega_{e} - \int_{\Omega_{e}} \psi_{i} S_{N}^{(e)} d\Omega_{e} = 0$$
Integration by parts:  

$$\int_{\Omega_{e}} \psi_{i} \nabla \cdot \mathbf{F}_{N}^{(e)} d\Omega_{e} = \int_{\Omega_{e}} \nabla \cdot (\psi_{i} \mathbf{F}_{N}^{(e)}) d\Gamma_{e} - \int_{\Omega_{e}} \nabla \psi_{i} \cdot \mathbf{F}_{N}^{(e)} d\Omega_{e} = \int_{\Gamma_{e}} \mathbf{n} \cdot \psi_{i} \mathbf{F}_{N}^{(e)} d\Gamma_{e} - \int_{\Omega_{e}} \nabla \psi_{i} \cdot \mathbf{F}_{N}^{(e)} d\Omega_{e} = \int_{\Omega_{e}} \nabla \psi_{i} \cdot \mathbf{F}_{N}^{(e)} d\Omega_{e} = 0$$

$$\int_{\Omega_{e}} \psi_{i} \frac{\partial \mathbf{q}_{N}^{(e)}}{\partial t} d\Omega_{e} + \underbrace{\int_{\Gamma_{e}} \mathbf{n} \cdot \psi_{i} \mathbf{F}_{N}^{(e)} d\Gamma_{e}}_{face integral} - \underbrace{\int_{\Omega_{e}} \nabla \psi_{i} \cdot \mathbf{F}_{N}^{(e)} d\Omega_{e}}_{volume integrals}$$

Matrix form:

$$\begin{split} M_{ij}^{(e)} \frac{\mathrm{d}\mathbf{q}_{j}^{(e)}}{\mathrm{d}t} &+ \sum_{f=1}^{N_{faces}} \left(\mathbf{M}_{ij}^{(e,f)}\right)^{T} \mathbf{F}_{j}^{(e,f,*)} - \left(\tilde{\mathbf{D}}_{ij}^{(e)}\right)^{T} \mathbf{F}_{ij}^{(e)} - S_{i}^{(e)} = 0\\ M_{ij}^{(e)} &= \int_{\Omega_{e}} \psi_{i} \psi_{j} \mathrm{d}\Omega_{e} \qquad \mathbf{M}_{ij}^{(e,f)} = \int_{\Gamma_{e}} \psi_{i} \psi_{j} \mathbf{n}^{(e,f)} \mathrm{d}\Gamma_{e} \qquad \tilde{\mathbf{D}}_{ij}^{(e)} = \int_{\Omega_{e}} \nabla \psi_{i} \psi_{j} \mathrm{d}\Omega_{e}\\ \max \text{ mass matrix} \qquad \text{face mass matrix} \qquad \text{differentiation matrix} \end{split}$$

# Unified CG/DG methods

$$\int_{\Omega_e} \psi_i \frac{\partial \mathbf{q}_N^{(e)}}{\partial t} d\Omega_e + \int_{\Gamma_e} \psi_i \mathbf{n} \cdot \mathbf{F}_N^{(*)} d\Gamma_e - \int_{\Omega_e} \nabla \psi_i \cdot \mathbf{F}_N^{(e)} d\Omega_e - \int_{\Omega_e} \psi_i \mathbf{S}_N^{(e)} d\Omega_e = \mathbf{0}$$

1. Evaluate "volume" integrals on element interiors

$$R^{(e)} := \int_{\Omega_e} \nabla \psi_i \cdot F_N^{(e)} d\Omega_e + \int_{\Omega_e} \psi_i S_N^{(e)} d\Omega_e$$
2. Evaluate flux integrals
$$R^{(e)} := R^{(e)} - \int_{\Gamma_e} \psi_i n \cdot F_N^{(*)} d\Gamma_e \quad \text{CG: cancels at interior element edges}$$
3. Direct Stiffness Summation
$$R = \bigwedge_{e=1}^{N_e} R^{(e)} \quad \text{DG: matrices are block diagor except for the flux matrix}$$

DG: matrices are block diagonal except for the flux matrix

4. Multiply by inverse global mass matrix and evolve time step

 $\frac{dq_i}{dt} = M_i^{-1}R_i$ 

We rely on inexact integration so M is diagonal

• NUMA carries CG and DG, xNUMA CG, and ATUM DG

## Flux-Difference DG methods

Have also been exploring flux-difference DG methods

> First consider that discrete integration by parts (SBP property) is satisfied by Lobatto points with inexact integration

$$\left(D_{ij} + D_{ij}^{T}\right)f_{j}^{(e)} = F_{ij}f_{j}^{(e)} \to \int_{x_{0}}^{x_{1}} \left(\psi f_{x} + \psi_{x}f\right)dx = [\psi f]_{x_{0}}^{x_{1}}$$

Such that row sum of D is zero:

$$\sum_{j=1}^{M_N} D_{ij} = 0$$

> This allows us to write Advection and Conservation forms in the same way (ignoring the boundary flux for simplicity)

$$M_i \frac{d\mathbf{q}_i^{(e)}}{dt} + D_{ij} \left( \mathbf{u}_k^{(e)} \mathbf{q}_j^{(e)} \right) = 0$$

where k=j yields conservation form and k=i advection form

## Flux-Difference DG methods

For conservation laws discretized as:



with, e.g., the kinetic-energy-preserving flux [4] being

$$\hat{f}_{ij}^{(adv)}(q,\mathbf{u}) = 2[[\mathbf{u}_i]]\{\{q_j\}\}, \quad \hat{f}_{ij}^{(con)}(q,\mathbf{u}) = 2\{\{\mathbf{u}_i\}\}\{\{q_j\}\}\$$

- and other options for entropy-stable flux [5]
- Let's see why this is important

# **Stabilizing EBG Methods**

Baroclinic Instability in a channel for 12-days using Grid Resolution: 100 km x 100 km x 1 km



- SE with hyper-viscosity (that needs to be tuned) yields similar results to DG with Kinetic-Energy-Preserving and Entropy-Stable flux (with no need to tune). All NUMA simulations are stable indefinitely.
- Conclusion: SE + Visc and DG KEP and ES offer stability with limited dissipation (good for hurricane RI); hyper-viscosity needs to be tuned. SE + Visc currently offers faster time-to-solution.

## <u>Multi-scale Methods</u>

- Recalling multi-scale methods (see [6]) we consider the following PDE
  - ▶  $\frac{\partial q}{\partial t} = S(q)$  where  $q = \bar{q} + \tilde{q}$  with  $(q, \bar{q}, \tilde{q})$ represent the total, coarse-scale, and fine-scale solutions; S(q) the RHS operator
- Using a VMS approach, we can decouple these (after some algebra) as

$$\begin{split} \int_{\Omega_e} \bar{\psi}_i \frac{\partial \bar{q}}{\partial t} d\Omega_e &= \int_{\Omega_e} \bar{\psi}_i \left( S(\bar{q}) - \frac{\partial \tilde{q}}{\partial t} + \frac{\partial S}{\partial q}(\bar{q}) \tilde{q} \right) d\Omega_e \\ \int_{\Omega_e^s} \tilde{\psi}_i \frac{\partial \tilde{q}}{\partial t} d\Omega_e^s &= \int_{\Omega_e^s} \tilde{\psi}_i \left( S(\bar{q}) - \frac{\partial \bar{q}}{\partial t} + \frac{\partial S}{\partial q}(\bar{q}) \tilde{q} \right) d\Omega_e^s \end{split}$$

Unlike classical VMS, here we computationally resolve coarse and fine scale solutions. However, we are currently first considering a simpler approach.



## <u>Multi-scale Methods</u>

Using the multi-scale modeling framework (MMF, see [7]) we consider the two PDEs

- ▶  $\frac{\partial Q}{\partial T} = S(Q) + F(Q,q)$  and  $\frac{\partial q}{\partial t} = s(q) + f(q,Q)$  where (Q,q) represent the coarsescale and fine-scale solutions, (S,s) the RHS operators, and (F,f) the coupling (forcing) between the coarse- and fine-scales
- Using a standard super-parameterization approach, we solve the two problems denoted as



Q: Coarse-Scale Model:

q: Fine-Scale Model:

Computational savings arises from elements only communicating at the Coarse-Scale model and at its larger time-step  $\Delta T = m \Delta t$ 

# MMF Result: Squall Line

#### Time: 0 sec



potential temperature clouds rain

#### Fine Simulation Standard (dX=200m)



## Superparameterization SP (dX=2km/ dx=100m)



#### Coarse Simulation Standard (dX=2km)

(mm/s)



#### 1000 0.040 Standard ( $\Delta X = 200 \text{ m}$ ) Standard ( $\Delta X = 2 \text{ km}$ ) 0.036 SP ( $\Delta X = 2 \text{ km}$ ) 100 0.032 0.028 Rain acc. (mm) 0.024 10 0.020 0.016 0.012 0.008 0.1 0.004 30 60 90 120 150 0 0.000 Horizontal distance (km)

#### Work by Soonpil Kang (NPS)

## **Time-Integration**

> The classical way to evolve CRM and LES in time are IMEX methods as follows:

▶  $\frac{dq}{dt} = \{S(q) - L(q)\}_{EX} + [L(q)]_{IM} \equiv S(q) + \mathcal{F}(q)$ , where L(q) is a linear operator that extracts the acoustic waves and allows us to partition the ODE into its slow and fast components  $(S, \mathcal{F})$ 

We have relied on s-stage Additive Runge-Kutta (SDIRK) methods:

$$P^{(i)} = q^{n} + \Delta t \sum_{j=1}^{i-1} a_{ij}^{E} \mathcal{S} \left( Q^{(j)} \right) + \sum_{j=1}^{i} a_{ij}^{I} \mathcal{F} \left( Q^{(j)} \right),$$

$$P^{n+1} = q^{n} + \Delta t \sum_{j=1}^{s} b_{i} S \left( Q^{(j)} \right)$$

Replacing  $\mathcal{F} \to \mathcal{N}$  where  $\mathcal{N}$  is a nonlinear operator is also possible but requires special care in solving (e.g., Newton's method, JFNK, etc.).

For many problems, standard IMEX may not be optimal. In particular, if the slow process is expensive to compute and the fast process inexpensive.

# <u>MMF + MR</u>

To understand why, let us first describe the current strategy used to evolve the MMF scheme:

1. 
$$Q^{n+1} = Q^n + \Delta t \left[ R(Q^{n+1}, q^n) \right]$$
,

2. 
$$q^{n+\frac{i}{m}} = q^{n+\frac{(i-1)}{m}} + \frac{\Delta t}{m} \left[ R(q^{n+\frac{i}{m}}, Q^{n+1}) \right], i = 1, ..., m$$





### MMF + MR

We propose a more consistent coupling using multirate (MR) (e.g., see [8]) as follows, where the stages are synchronized. The stage values are given as

1. 
$$Q^{(j^{O})} = Q^{n} + \Delta t \sum_{k=1}^{j^{O}-1} a_{j^{O},k}^{O} R\left(Q^{(j^{O})}, q^{(*)}\right),$$

2. 
$$q^{(i^{I},j^{O})} = q^{(1,j^{O})} + \left(c_{j^{O}}^{O} - c_{j^{O}-1}^{O}\right) \Delta t \sum_{k=1}^{i^{I}-1} a_{i^{I},k}^{I} R\left(q^{(k,j^{O})}, Q^{(*)}\right),$$

3. 
$$q^{(j^{O})} = q^{(1,j^{O})} + \tilde{c}_{j^{O}}^{O} \Delta t \sum_{i=1}^{s^{I}} b_{i}^{I} R\left(q^{(i,j^{O})}, Q^{(*)}\right),$$

4. 
$$Q^{(j^{O})} = Q^{n} + \Delta t \sum_{i=1}^{s^{O}} b_{i}^{O} R\left(Q^{(i)}, q^{(i)}\right)$$

Some concerns: MIS [8] executes MR across stages and is general tableau indicates a likely issue with conservation of linear invariant: MPRK [9] allows for conservation but limited to the same fast/slow method. This approach is certainly better than the standard approach but will it be too expensive?



#### 3-stage 2-Rate Fast Tableau

# **Multirate Time-Integration**

Let us consider the baroclinic instability on the 3-sphere using ARK1 for hyper-diffusion and 1D-IMEX ARK2 for the remaining operators.



- Multirate yields 30% increase in performance over singlerate 1D-IMEX-ARK2 (which we know already scales well). We have yet to exploit all possibilities offered in:
  - 1. Patrick Mugg, Extrapolated Multirate Methods for Hyperbolic Partial Differential Equations, NPS PhD Thesis (June 2021); paper in preparation
  - 2. Alves, Kelly, Giraldo, Implicit time-integrators for global nonhydrostatic atmospheric modeling (in preparation)

#### IMEX: No-Schur vs Schur Form

For the shallow water equations:

 $\phi_t + \nabla \cdot \mathbf{U} = 0$  $\mathbf{U}_t + \nabla \phi = 0$ 

Discretizing in both space (via strong form CG) and time (assume ARK1) results in the No-Schur form:

 $M\phi^{n+1} + \Delta t \mathbf{D}^T \mathbf{U}^{n+1} = M\phi^n$  $M\mathbf{U}^{n+1} + \Delta t \mathbf{D}\phi^{n+1} = M\mathbf{U}^n$ 



Applying a block LU factorization (or subbing U<sup>n+1</sup> into 
$$\phi^{n+1}$$
 equation) yields the Schur form:

$$M\phi^{n+1} - \Delta t^2 \mathbf{D}^T M^{-1} \mathbf{D} \phi^{n+1} = R^n$$

A few observations: 1) we need  $M^{-1}$ ; 2) This system is smaller ( $\mathcal{O}(N^2)$  instead of  $\mathcal{O}(N_{var}N)^2$ ); 3) better conditioned [10].

10] F.X. Giraldo, M. Restelli, and M. Laeuter, Semi-implicit formulations of the Euler equations: applications to nonhydrostatic atmospheric modeling, SIAM J. Sci. Comp., Vol. 32, 3394-3425 (2010)

## IMEX: No-Schur vs Schur Form

For general systems of equations we write (after integration by parts):

$$\int_{\Omega_e} \psi_i \frac{\partial \mathbf{q}^{(e)}}{\partial t} d\Omega_e + \int_{\Gamma_e} \psi_i \mathbf{n} \cdot \mathbf{F}^{(*)} d\Gamma_e - \int_{\Omega_e} \nabla \psi_i \cdot \mathbf{F}^{(e)} d\Gamma_e = \int_{\Omega_e} \psi_i \mathbf{S}^{(e)} d\Omega_e$$

Writing the numerical fluxes as:

$$\mathbf{F}^{(*)} = \{\{\mathbf{F}\}\} - \frac{\lambda \mathbf{n}}{2}[[\mathbf{q}]] \longrightarrow \int_{\Gamma_e} \psi_i \mathbf{n} \cdot \mathbf{F}^{(*)} d\Gamma_e = \mathbf{C}_G^T \mathbf{F} - \mathbf{J}_G^T \mathbf{q}$$

Discretizing in space (via EBG) yields:

$$M\frac{d\mathbf{q}}{dt} + \mathbf{C}^T\mathbf{F} - \mathbf{J}^T\mathbf{q} - \mathbf{D}^T\mathbf{F} = S$$

Discretizing in time (via ARK1) yields:  $(M - \Delta t \mathbf{J}) \mathbf{q}^{n+1} + \Delta t [\mathbf{C}^T \mathbf{F} - \mathbf{D}^T \mathbf{F} - S]^{n+1} = M \mathbf{q}^n$ 

If J non-empty then no longer block diagonal so computing  $(M - \Delta t \mathbf{J})^{-1}$  is non-trivial

Why this matters: To construct the Schur complement, we need to isolate terms from one equation to substitute into another. To do this, we need to invert the mass matrix

#### IMEX: No-Schur vs Schur Form

For DG we can avoid this difficulty by separating Linear and Nonlinear fluxes:

$$\int_{\Omega_e} \psi_i \frac{\partial \mathbf{q}^{(e)}}{\partial t} d\Omega_e + \int_{\Gamma_e} \psi_i \mathbf{n} \cdot (\mathbf{F}_L + \mathbf{F}_{NL})^{(*)} d\Gamma_e - \int_{\Omega_e} \nabla \psi_i \cdot (\mathbf{F}_L + \mathbf{F}_{NL})^{(e)} d\Gamma_e = \int_{\Omega_e} \psi_i \mathbf{S}^{(e)} d\Omega_e$$

Which we write in matrix-vector form:

$$\left(M - \Delta t \mathbf{J}_L\right) \mathbf{q}^{n+1} + \Delta t \left(\mathbf{C}^T - \mathbf{D}^T\right) \mathbf{F}_L^{n+1} = \left(M + \Delta t \mathbf{J}_{NL}\right) \mathbf{q}^n - \Delta t [S + \left(\mathbf{C}^T - \mathbf{D}^T\right) \mathbf{F}_{NL}]^n$$

Flux Choices: If  $\mathbf{J}_L = 0$  then we can easily isolate  $\mathbf{q}^{n+1}$ 

With the proper selection of fluxes [11] we can construct a stable DG Schur form.

#### IMEX: DG Schur Form

No-Schur Form:  $\rho_{tt} = \hat{\rho} - \alpha \nabla \cdot \mathbf{U}_{tt}, \quad \mathbf{U}_{tt} = \hat{\mathbf{U}} - \alpha \left( \nabla P_{tt} + \rho_{tt} \nabla \phi \right)$ 

$$E_{tt} = \hat{E} - \alpha \nabla \cdot (h_0 \mathbf{U}_{tt}), \qquad P_{tt} = (\gamma - 1)(E_{tt} - \rho_{tt}\phi)$$

Schur Form for Pressure (plugging  $\rho_{tt} \rightarrow \mathbf{U}_{tt} \rightarrow E_{tt}$ ):

$$P_{tt} - \alpha^2 (\gamma - 1) [\nabla \cdot (h_0 \mathbf{L}) - \phi \mathbf{L}] = (\gamma - 1) [\hat{E} - \phi \hat{\rho} - \alpha (\nabla \cdot (h_0 \mathbf{R}) - \phi \nabla \cdot \mathbf{R})]$$

$$\mathbf{L} = A^{-1} [\nabla P_{tt} + \frac{G}{\gamma - 1} P_{tt})], \qquad \mathbf{R} = A^{-1} [\hat{\mathbf{U}} - \alpha \mathbf{G} (h_0 \hat{\rho} - \hat{E})] \qquad A = \mathbf{I} + \alpha^2 \mathbf{G} \nabla h_0$$

Properties of Schur Form: all eigenvalues are real and positive (SPD as expected for a Helmholtz operator), see [11].



[11] S. Reddy, M. Waruszewski, F.A.V. B. Alves, F.X. Giraldo, IMplicit-EXplicit formulations for discontinuous Galerkin non-hydrostatic atmospheric models, JCP (in revision, May 2023)

## IMEX: DG Schur Form



### <u>Summary</u>

- EBG offers elegant way to approximate spatial derivatives of PDEs.
  - EBG methods offer much flexibility: geometric and algorithmic.
  - Schur forms offer an increase in performance as stand-alone methods or as preconditioners for more sophisticated methods (e.g., nonlinear IMEX).
- Flux-Differencing perform well under the stability metric but are computationally expensive (ES is 10x more expensive than hyper-diffusion and KEP is 5x due to a variety of reasons such as the time-step restriction and number of FLOPS).
- Combing Flux-Differencing DG with Schur forms is appealing.

## <u>Summary</u>

- Our MMF model (xNUMA) is able to launch one CRM with an arbitrary number of LES models in both 2D and 3D.
  - Completed work: squall line test with warm rain [12].
  - Future work: Hurricane simulations with moisture (benchmark simulations in progress).
- Currently, CRM uses MPI. N LES runs:
  - use N MPI ranks to exploit hardware peak performance.
  - will use GPUs (work in progress).
  - Multirate time-integration offers a high-order, consistent, elegant, and powerful way to solve MMF problems.



