Development of a Nodal DG Solver within the SU2 Framework

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Outline

• Motivation for high-order schemes
• DG-FEM, the basic principles
• Current solver capabilities
• Access, compile and run the code
• Main DG-solver routines
• Time-accurate local time stepping
• Conservative vs. entropy variables
• Shock capturing
• LES models
• Performance optimization
Why do we need high-order schemes?

$2^{nd}$ order schemes have been extremely successful, certainly for RANS. SU2 FV is used for many applications...
But...

For some applications 2\textsuperscript{nd} order accuracy may not be sufficient

Examples

- Wake and vortex flows
- Noise prediction
- DES/LES/DNS

DG solver is intended for high-fidelity modeling of the turbulence, i.e. LES (wall resolved and wall modeled) and DNS
Nodal DG-FEM: the basic principles (1)

Element $k$: $U(x_i) = \sum_{j=1}^{N_p} U^k_j \phi^k_j(x_i)$

Hyperbolic system of PDE’s
Weak formulation

$$\frac{\partial U}{\partial t} + \frac{\partial F_i}{\partial x_i} = 0 \quad \Rightarrow$$

$$\iint_{V_k} \frac{\partial U}{\partial t} \phi^k_m \, dV - \iint_{V_k} F_i \frac{\partial \phi^k_m}{\partial x_i} \, dV + \oint_{\partial V_k} F_i n_i \phi^k_m \, d\Omega_k = 0, \quad m = 1, \ldots, N_p$$

Integrals are computed with high enough accuracy to prevent instabilities due to aliasing errors
Nodal DG-FEM: the basic principles (2)

Contribution from the contour integral

Solution at the interfaces is multiply defined and discontinuous

\[ \int_{\partial V_k} F_i n_i \phi_m^k \, d\Omega_k \Rightarrow \int_{\partial V_k} F_i (U_L, U_R) n_i \phi_m^k \, d\Omega_k \]

Riemann problem: Any approximate Riemann solver can be used => stabilizes the discretization

1\textsuperscript{st} order DG-FEM equals 1\textsuperscript{st} order FVM!!!
Higher-order Grids with Curved Elements

In-house capability to generate higher-order grids for simple cases

A lot more effort should be put into high-order grid generation.
Current Capabilities

• Both 2D and 3D, just like SU2-FV
• All standard elements (tri, quad, tet, pyra, prism, hex)
• Curved elements of arbitrary order
• Arbitrary polynomial order solution elements
• Polynomial order can differ in individual elements
• Symmetric Interior Penalty method for viscous fluxes
• Explicit time integration schemes (Runge-Kutta type)
• Time-accurate local time stepping via ADER-DG
• Task scheduling approach for efficient parallelization
• Preliminary implementation of LES models and shock capturing
Access the code

- *feature_hom* branch on GitHub is the main branch for the DG solver
- Several other development branches exist
Compile the code

- configure script, like the rest of SU2
- Some additional flags are required, for handling of matrix multiplications
  - Native implementation (use for debugging only)
  - System BLAS/LAPACK routines
  - Intel MKL
  - LIBXSMM (available on GitHub)

```bash
FLAGS="-fpic -O2 -funroll-loops -ftree-vectorize -ffast-math"
FLAGS="$FLAGS -DHAVE_LIBXSMM"
INCFLAGS="-I$LIBXSMM_include_dir"
LDFLAGS=
LIBFLAGS="$LIBFLAGS $LIBXSMM_lib_dir/libxsmm.lib -lopenblas -lmsmpi -static -limagehlp"
CFLAGS="$FLAGS"
CXXFLAGS="$FLAGS -std=c++11"

cd $SU2_dir

build_cmd="./configure --enable-mpi --enable-tecio --with-cc=gcc --with-cxx=g++ CXXFLAGS=""$CXXFLAGS $INCFLAGS" CFLAGS="$CFLAGS $INCFLAGS" LDFLAGS="$LDFLAGS" LIBS="$LIBFLAGS" --with-metis-cppflags=""-O3" --with-parmetis-cppflags=""-O3" --prefix=$INSTALL_DIR --exec-prefix=$INSTALL_DIR"
```
Run the code

- Either sequential or parallel via mpirun (mpiexec)
- Additional parameters must be specified in the .cfg file
- Running via python should be possible, but currently no benefit (no multi-disciplinary applications yet)
Main DG-solver routines

- **Partitioning**
  - Common/src/geometry_structure_fem_part.cpp
  - Common/src/fem_work_estimate_metis.cpp

- **Preprocessing**
  - Common/include/fem_geometry_structure.hpp
  - Common/include/fem_standard_element.hpp
  - Common/src/fem_geometry_structure.cpp
  - Common/src/fem_integration_rules.cpp
  - Common/src/fem_standard_element.cpp

- **Solver**
  - SU2_CFD/include/solver_structure.hpp
  - SU2_CFD/src/integration_time.cpp
  - SU2_CFD/src/solver_direct_mean_fem.cpp
  - Common/src/dense_matrix_product.cpp
Time-accurate local time stepping

- Explicit schemes: Global time step determined by smallest element
- Inefficient when element sizes differ significantly
- Solution: time-accurate local time stepping
- Difficult (impossible?) for Runge-Kutta schemes
- Possible with space-time formulations, e.g. ADER-DG
- Practical restrictions
  - Only finite number of time steps allowed, which differ by a factor 2, i.e. $\Delta t$, $2\Delta t$, $4\Delta t$, etc.
  - Neighboring elements: max. one time level difference
- Challenge for the load balancing => task scheduler
Conservative vs. entropy variables

- Numerical stability can only be proven for symmetric systems
- Not the case for Navier-Stokes equations
- However, NS can be *symmetrized* using entropy variables

\[
B \frac{\partial v}{\partial t} + A_i \frac{\partial v}{\partial x_i} - \frac{\partial}{\partial x_i} \left( K_{ij} \frac{\partial v_j}{\partial x_j} \right) = 0
\]

\[
B = \frac{\partial F_i}{\partial v}, \quad A_i = \frac{\partial Q}{\partial v}, \quad Q : \text{Cons. variables}
\]

- Leads to an implicit formulation, even for explicit schemes
Shock capturing

- Shock capturing consists of two components:
  - Detecting the discontinuity
  - Resolving the discontinuity
- Detecting the discontinuity:
  - Persson and Peraire: Modal decay
  - Clain, Diot and Loubere: MOOD
- Resolving the discontinuity
  - Limiter
  - Artificial viscosity / filtering
  - Sub-cell limiting
Shock capturing

- Sod’s shock tube problem
  - MOOD sensor
  - Sub-cell limiting

- MOOD sensor
- Filtering

\[ \text{Density}(\rho) \text{ at } T = 0.2, p_{\text{space}} = 4, p_{\text{time}} = 1, N_{\text{Elem}} = 100, \text{CFL} = 0.4 \]
LES Models

• SGS Models
  – Constant Smagorinsky
    \[ \nu_{sgs} = C_s^2 \Delta^2 |\bar{S}| \]
  – Wall-Adapting Local Eddy Viscosity (WALE)
    \[ \nu_{sgs} = (C_w \Delta)^2 \frac{(S_{ij} S_{ij})^{(3/2)}}{(S_{ij} S_{ij})^{(5/2)} + (S_{ij} S_{ij})^{(5/4)}} \]
  – More sophisticated models to be implemented in future
    • Dynamic Smagorinsky, etc.

• Wall Models
  – One-dimensional Equilibrium BL Equations
    \[ \frac{d}{dy} \left[ (\mu - \mu_t) \frac{d\bar{u}_||}{dy} \right] = 0 \]
    \[ \frac{d}{dy} (\bar{p}) = 0 \]
    \[ \frac{d}{dy} \left[ \bar{u}_|| (\mu + \mu_t) \frac{d\bar{u}_||}{dy} + \left( \frac{\mu c_p}{P_r} + \frac{\mu_t c_p}{P_{rt}} \right) \frac{dT}{dy} \right] = 0 \]
Performance optimization

• First implementation was very inefficient (< 5% peak on Xeon)

• Collaboration with Intel to improve efficiency
  ▪ Specialized matrix multiplication software (BLAS, LIBXSMM)
  ▪ Explicit unrolling of small loops (specialized 2D, 3D code)
  ▪ Vectorization direction matrix multiplication: 128 byte aligned
  ▪ Element-wise operation fusion for vectorization

• Current performance: ≈ 40% peak on Xeon

• Thoughts about hybrid MPI-OpenMP to increase flexibility

• Potential for advanced (Regent/Legion) methods to help scalability and portability
Strong scaling test on Theta (ANL)

Strong scaling test - SD7003, 0.49M Elem, p = 4, Hexs

<table>
<thead>
<tr>
<th>Elem/Rank</th>
<th>0.25M</th>
<th>0.12M</th>
<th>30.7K</th>
<th>7.68K</th>
<th>1.92K</th>
<th>480</th>
<th>120</th>
<th>30</th>
</tr>
</thead>
<tbody>
<tr>
<td>DOF/Rank</td>
<td>30.7M</td>
<td>15.4M</td>
<td>3.84M</td>
<td>0.96M</td>
<td>0.24M</td>
<td>60K</td>
<td>15K</td>
<td>3.75K</td>
</tr>
<tr>
<td>Efficiency(%)</td>
<td>N/A</td>
<td>99.98</td>
<td>97.15</td>
<td>90.89</td>
<td>93.39</td>
<td>90.49</td>
<td>85.07</td>
<td>77.86</td>
</tr>
</tbody>
</table>
Results ($p = 4$, triangles, inviscid)
Visualization via linear sub-elements
Results, inviscid
Visualization via linear sub-elements

\[ p = 3, \text{ tets} \]

\[ p = 4, \text{ triangles} \]
Results, viscous
Implicit LES, SD 7003 (Reynolds = 60,000)

\( p = 4, \) hexahedra
Work to be done

• Thorough V&V of the implementation
• Finish shock capturing
• Finish LES wall models
• LES statistics (common to DDES and URANS)
• Improve boundary conditions (non-reflective)
• Performance optimization, including OpenMP parallelization
• Grid motion, sliding mesh interfaces
• Grid sequencing
• High-order grid generation