RPSVV Working group outbrief

Robustness, Performance, Scalability, Verification, & Validation

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SU2

Key initiatives

- **Robustness**: *reliably getting a solution with minimal tuning*
- **Performance & Scalability**: *improving time-to-solution, including massively parallel situations*
- **Verification & Validation**: *ensure we rigorously solve the equations correctly (verification) and that we solve the correct equations for the physical phenomena of interest (validation)*

Key initiatives

- **Robustness**: *reliably getting a solution with minimal tuning*
  - Multigrid not robust and rarely used for viscous calculations
    - RANS agglomeration could be improved for anisotropic grids (and based on grid quality)
    - Action point: look at agglomeration strategy, including directional coarsening
  - Convergence issues /stalling residuals due to spatial discretization
    - Assess currently available limiters and see which work well. Edge based vs cell based?
    - Action item: look at different limiters and strategies not yet implemented in SU2
    - Test cases from Matteo are available that demonstrate typical convergence issues
    - Alberto has a limiter implementation that can be ported/tested
    - Action item: compute grid metrics, write out to console (e.g., show min/max) and look at “limiting” limiters or fixing problem cells based on quality (Eduardo)
    - Action item: look at error of GG and WLS using MMS framework, i.e., differentiate manufactured solution and compute error.
    - Action item: look at new gradient calculation techniques
    - Make sure to check for these problems on non-smooth grids in 3D

Key initiatives

- **Robustness**: *reliably getting a solution with minimal tuning*
  - Linear solver / Jacobian improvements to help convergence
    - Consider exact Jacobians? Is it worth the cost (development time, memory) for segregated RANS approach?
    - Action item: look at improving Jacobians - Pedro has some ideas for some improvements
    - Pedro interested in adding something for small data structures / matrix storage for clarity and performance (eigen?)
    - Many convective schemes do not have consistent Jacobians
    - Check whether Jacobians at boundary conditions, or inconsistent weak convective flux for BC, are causing any issues

Key initiatives

- **Performance & Scalability**: *improving time-to-solution, including massively parallel situations*
  - Preprocessing of large grids contains a bottleneck around 100M cells
    - ASCII not possible at scale
    - Options: stick with CGNS (serial or parallel) or have our own binary format for large grids
    - CGNS serial has some current limitations, but possible fix just released in v3.4
    - CGNS parallel can be difficult to install due to dependencies
    - Major drawbacks of creating our own format:
      - We need to develop and support converters or convince mesh packages to export a new binary format (e.g., maybe have CGNS carry a converter)
      - Creates roadblock for people that have existing workflows that rely on CGNS already
    - See how this affects the other working groups and ask for other format suggestions
    - Action items: (1) try the serial CGNS fix, (2) try parallel CGNS, (3) create our own binary format
  - ADT collects all surface nodes on each rank which will eventually be a memory issue on very large grids
    - Parallel ADT is possible but performance could be poor
    - Could try eikonal equation for distance search instead of ADT (PDE-based approach)
    - Possible option of a hybrid ADT approach to combine serial/parallel approaches
    - Another a bottleneck is that the master rank processes all markers from the grid in the FVM solver currently, but this should be a straightforward fix

Key initiatives

- **Performance & Scalability**: *improving time-to-solution, including massively parallel situations*
  - Hybrid OpenMP-MPI strategy
    - We have done this for the FVM solver but exists only in a special branch (see).
    - Could be useful to improve strong scaling by using one rank per socket and then using threading on each core per socket which leads to larger MPI partitions (but requires a second-level partitioning on each rank for OpenMP threads).
    - Could reach more Windows users with this implementation
    - Would postpone the ADT search issue until much larger grids
    - Is also interesting for DG with the ADER scheme due to available task handling in OpenMP
    - CoDi should be able to handle it if we create an OpenMP wrapper that is similar to the current MPI wrapper in SU2
    - Drawbacks: adds complexity for developers, makes the code less readable, and would need a new wrapper for AD support
    - Important to make sure the user always has a working out of the box configuration
  - Multizone parallelization: even partitioning of each zone leads to major communication issues on small zones and lack of convergence
    - Action item: split communicators so that we can avoid communication penalties and performance issues by over-partitioning
    - Need to take care with load balance issues
    - Communicate with MDAO group about these changes, especially transfers (Ruben)

Key initiatives

- **Performance & Scalability**: *improving time-to-solution, including massively parallel situations*
  - Data structures could be more efficient, including locality
    - Array-of-structures is a know issue with memory locality (see “Performance optimizations for scalable implicit RANS calculations with SU2”), can move to structures-of-arrays if it does not remove too much flexibility/readability
    - Max offered take a look at data structures
  - Future architectures / accelerators (for future, not discussed at 4th meeting)
    - Keep an eye on evolving hardware for many-core, GPU, FPGA, etc.
    - Consider new algorithms that map best to architectures
    - Ensure we maintain flexibility to adapt to new paradigms in the future (might be driven by AI market, for instance)

Key initiatives

- **Verification & Validation**: *ensure we rigorously solve the equations correctly (verification) and that we solve the correct equations for the physical phenomena (validation)*
  - Perform Galilean invariance checks to verify ALE problems
  - RANS MMS case must be added
  - Add MMS cases for BCs as well (e.g., periodic, mixing plane, ?)
  - Ensure MMS solutions always balance terms in the PDE
  - Request: make sure config option for user-defined solution is separate from the “verification” for clarity
  - Wind turbine validation case(s) from Huseyin
  - Validation template to be proposed by Alberto, possibly organized by applications for the validation
  - Challenge cases: turbomachinery, including possible turbine case from Bosch (Piero/Matteo)

Envisioned Required Code Developments

- Improvements to existing geometric multigrid (FAS) or new multigrid algorithm(s)
- New limiters/reconstruction/grid checks for robust convergence
- Linear solver/Jacobian improvements for robust convergence
- Fixes for existing CGNS reader or new native binary format for large grids (>100M cells)
- Algorithmic enhancements for massively parallel searches (ADT or otherwise)
- Devise a strategy for potential hybrid OpenMP-MPI implementation
- Optimize data structures for performance while balancing readability/flexibility
- Improve parallelization for multizone problems
- Expand MMS library to cover more governing equations, BCs, etc.

Working group members and commitments

- Multigrid -> Akshay
- Limiters/Reconstructions -> Eduardo, Salvo (if available), Tom, Alberto
- Jacobians / Data Structure Optimization -> Pedro, Max
- Grid Formats -> Tom, Edwin
- ADT -> Tommaso, Edwin
- Hybrid OpenMP-MPI Strategy -> Pedro, Max, Edwin
- Multizone Parallelization -> Salvo (if available), MDAO representative (?)
- V&V -> Alberto (submits a first proposal for format in V&V repo), Huseyin (considers entire test case framework planning, look at benchmark guidelines for AIAA for instance), Jayant (if available)

Point(s) of contact

Primary PoCs:
Edwin van der Weide
Thomas Economon

Participants at 4th Meeting:
Edwin van der Weide
Tommaso Bellosta
Camilla Conti
Pedro Gomez
Matteo Pini
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Email addresses on request