Explicit Discontinuous Galerkin Schemes for Direct and LES Simulations

Gregor Gassner, Frieder Lörcher, Claus-Dieter Munz

gassner@iag.uni-stuttgart.de

Institut for **A**erodynamics and **G**asdynamics

University of Stuttgart

Overview

- Diffusion
- Nodal Integration
- Space-time expansion
- Results

Diffusion I

- Scalar linear heat equation

$$u_t - \Delta u = 0 \tag{1}$$

- Standard approach
  - Resorting to a first order system (Bassi&Rebay 1997)

$$\begin{aligned} u_t - \nabla \cdot \mathbf{q} &= 0 \\ \mathbf{q} - \nabla u &= 0 \end{aligned} \tag{2}$$

  - 'Classic' weak formulation for extended system
  - We need numerical approximation of the solution u and $\mathbf{q}$ at grid cell boundaries
  - For 3D comp. NSE: 15 auxiliary variables are needed

Diffusion II

- Our approach
  - Use the original second order equation
  - Classic weak formulation

$$\begin{aligned} \langle u_t , \phi \rangle_Q &= \langle \Delta u, \phi \rangle_Q \,, \\ \langle u_t , \phi \rangle_Q &= (\nabla u \cdot \mathbf{n}, \phi)_{\partial Q} - \langle \nabla u, \nabla \phi \rangle_Q \end{aligned} \tag{3}$$

  - second integration by parts ('ultra' weak formulation)

$$\langle u_t , \phi \rangle_Q = (\nabla u \cdot \mathbf{n}, \phi)_{\partial Q} - (u, \mathbf{n} \cdot \nabla \phi)_{\partial Q} + \langle u, \Delta \phi \rangle_Q \tag{4}$$

  - New term strong related to symmetric term in SIP scheme (Nitsche 1971)
  - no auxiliary variables
- Can be generalized to non-linear systems if viscous terms have the structure

$$U_t = \nabla \cdot \mathbf{F}(U, \nabla U) = \nabla \cdot (\underline{D}(U) \nabla U) \tag{5}$$

Diffusion III

- We need approximation of u and $\nabla u \cdot \mathbf{n}$ at grid cell boundary
  - Diffusive generalized Riemann problem (dGRP)

$$
\begin{aligned}
&u_t - u_{xx} = 0, \\
&u(x, t=0) = \begin{cases} u^- + x u_x^- & \text{for } x < 0, \\ u^+ + x u_x^- & \text{for } x > 0 \end{cases}
\end{aligned} \tag{6}
$$

  - dGRP solution yields numerical approximation

$$
u_x\big|_{\partial Q} \approx \eta \frac{[\![u]\!]}{\Delta x} + \{u_x\} \quad \text{and} \quad u\big|_{\partial Q} \approx \{u\} \tag{7}
$$

  - Strong relation to the SIP scheme
  - η is a known quantity (depends on the order of the DG polynomial)

Diffusion IV

- Extension to non-linear diffusion systems

$$U_t - (\underline{D}(U)U_x)_x = 0 \tag{8}$$

  - Linearization of the diffusion matrix

$$\underline{D}(U) \approx \widetilde{\underline{D}} := \underline{D}(\{U\}) \tag{9}$$

  - Diagonalization of $\widetilde{\underline{D}}$ ('characteristic' variables)
  - Eigenvalues of $\widetilde{\underline{D}}$ are the diffusion coefficients of the decoupled system
  - Use dGRP solution for each of the scalar heat equations
  - Back transformation to conservative variables yields dGRP approximation

$$\underline{D}(U)U_x\big|_{\partial Q} \approx \widetilde{\underline{D}}\left(\eta\frac{[\![U]\!]}{\Delta x} + \{U_x\}\right) \quad \text{and} \quad U\big|_{\partial Q} \approx \{U\} \tag{10}$$

Diffusion V

- SIP approach (Hartmann et al. 2006)

$$\underline{D}(U)U_x\Big|_{\partial Q} \approx \eta_{SIP}\lambda_{max}\frac{[\![U]\!]}{\Delta x} + \{D(U)U_x\} \quad \text{and} \quad U\Big|_{\partial Q} \approx \{U\} \tag{11}$$

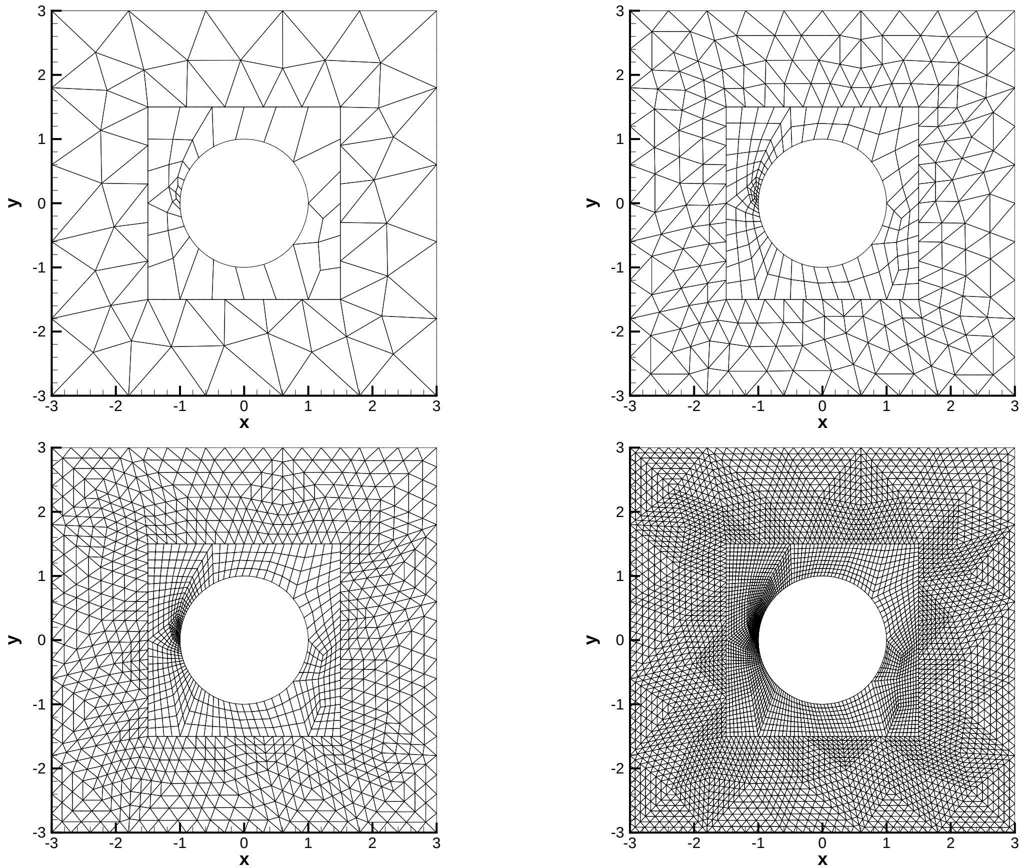
  - For advection diffusion problems with semi definite diffusion matrix

$$EOC_{SIP} = \begin{cases} p+1 & \text{for } p \text{ odd} \\ p & \text{for } p \text{ even} \end{cases} \tag{12}$$

- Compressible NSE (no diffusion in density equation)
  - SIP problem: density jump penalty in density equation
  - dGRP solution: if we multiply jump term with diffusion matrix, no direct penalty term in density equation
    $\Rightarrow$dGRP approach yields optimal *EOC* for comp. NSE equations
- we tested several semi definite advection diffusion systems with same result

Diffusion VI

- EOC for compressible Navier-Stokes equations
  - grid sequence with triangles, quadrilaterals, hanging nodes and curved elements for h-convergence



Diffusion VII

- Exact analytical solution
  - Choose smooth analytical function
  - Insert function into comp. NSE
  - Use right hand side as source term
  - Solve inhomogeneous comp. NSE

- Results

	$\mathbf{L_2}(\rho\mathbf{e})$	**EOC**	$\mathbf{L_2}(\rho\mathbf{e})$	**EOC**
refinement	**p=4**		**p=5**	
0	$1,02E-02$	**-**	$2,91E-03$	**-**
1	$3,48E-04$	**4,9**	$7,31E-05$	**5,3**
2	$1,29E-05$	**4,8**	$1,07E-06$	**6,1**
3	$4,13E-07$	**5,0**	$1,65E-08$	**6,0**

Nodal Integration I

- We choose a modal polynomial representation to simplify p-adaption, modal filtering and explicit time stepping. Furthermore, orthogonal hierarchical polynomial trial function are well suited for VMS scale separation.
- Problem: evaluation of the integrals
  - L_2 stability, if integrals computed exactly: not possible for comp. NSE
  - No loss of EOC, if integral evaluation is exact for linear problems
  - Standard approach: numerical integration (Gauss)

$$\left\langle f_1(u), \frac{\partial \phi}{\partial x_1} \right\rangle_Q \approx \sum_{j=1}^{(p+1)^d} f_1(u(\chi_j)) \frac{\partial \phi}{\partial x_1}(\chi_j)\omega_j \qquad (13)$$

  - Gauss points do not lie on the grid cell surface, therefore can not be reused for surface integral
  - Example: $p = 5$ hexahedron needs 216 cubature points for volume integral and 216 cubature points for surface integral ($= 432$ flux evaluations)

Nodal Integration II

- Our approach: Nodal integration
  - Interpolate pth order polynomial of the non-linear flux f
  - Insert into integral and (pre-)integrate exactly

$$\left\langle f_1(u), \frac{\partial \phi}{\partial x_1} \right\rangle_Q \approx \sum_{i=1}^{N} f_1(u(\xi_i)) \left\langle \psi_i, \frac{\partial \phi}{\partial x_1} \right\rangle_Q \qquad (14)$$

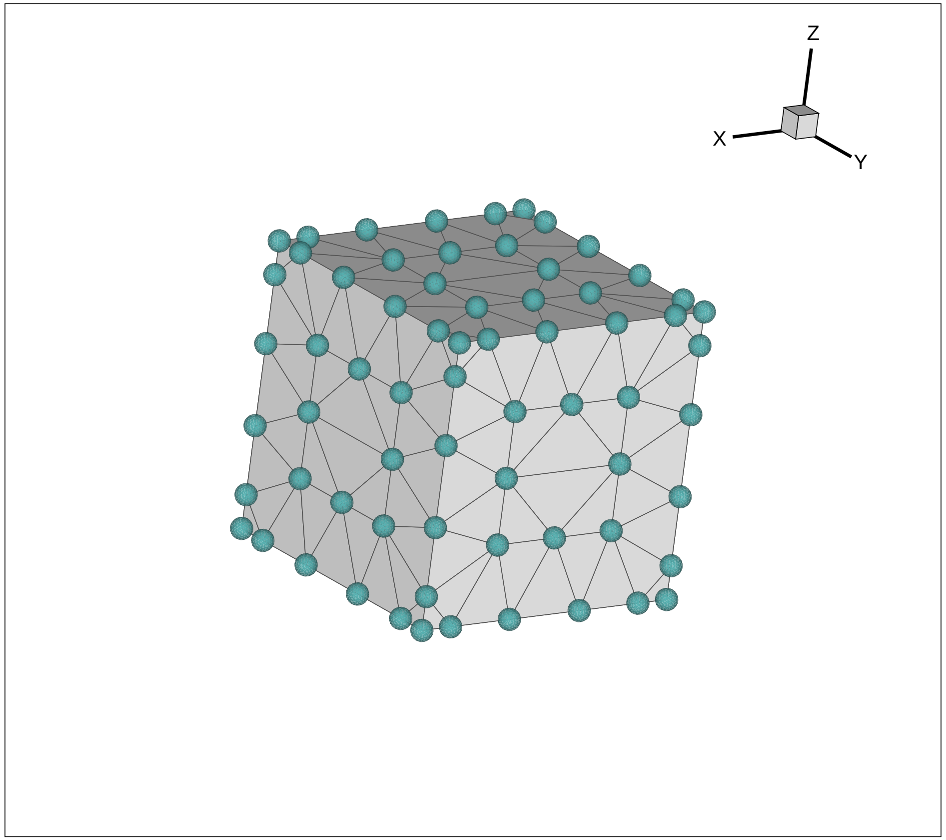
  - number of interpolation points

$$N_{min} = \frac{(p+d)!}{d!p!} \leq N \leq N_{max} = (p+1)^d \qquad (15)$$

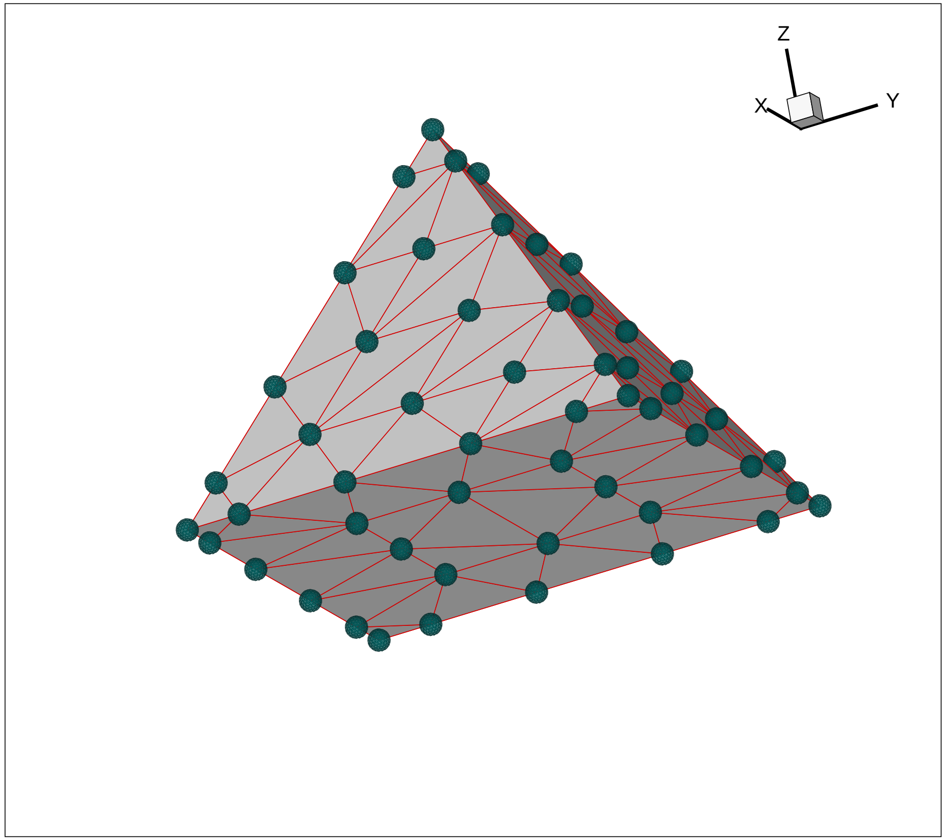
  - we can choose int. points that simultaneous support a pth order accurate interpolation on the surface
  - Example: Interpolation for $p = 5$ hexahedron with $N = 105$ points (432 flux evaluations for Gauss approach)

Nodal integration III

- Interpolation points for $p = 5$.



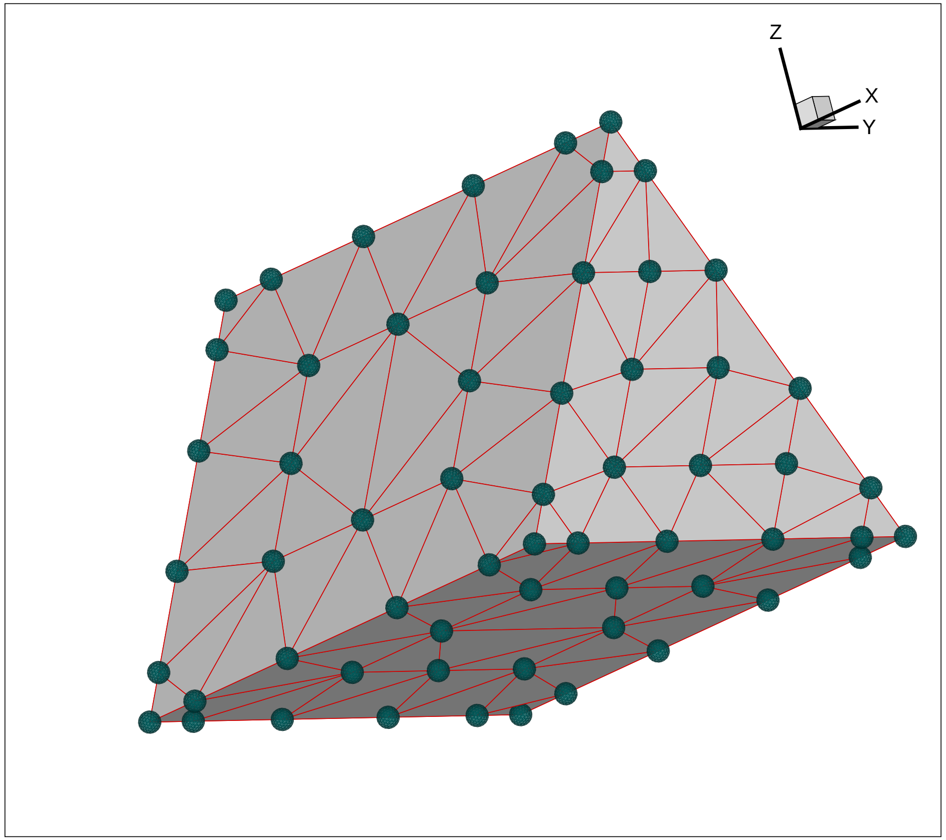
hexahedron with $N = 105$



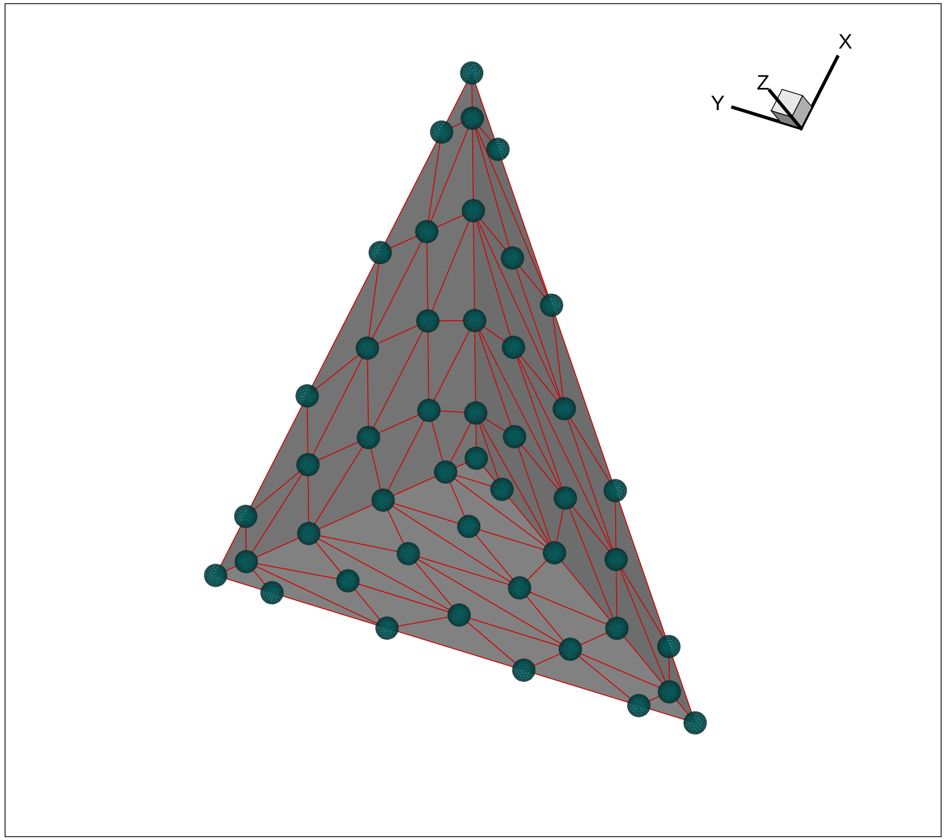
pyramid with $N = 74$

Nodal integration IV

- Interpolation points for $p = 5$.



pentahedron with $N = 84$



tetrahedron with $N = 56$

Space Time Expansion I

- As we aim to perform large scale computations on massive parallel clusters, we decided to use an explicit time discretization to fully utilize the locality of the DGM
  - Semi discrete DG formulation

$$\langle u_t, \phi \rangle_Q = \underbrace{S(u^{\pm}, \nabla u^{\pm})}_{\text{surface terms}} + \underbrace{V(u, \nabla u)}_{\text{volume terms}} \tag{16}$$

  - We simple integrate (16) from time level t_n to t_{n+1}

$$\left\langle u^{n+1}, \phi \right\rangle_Q = \langle u^n, \phi \rangle_Q + \int_{t_n}^{t_{n+1}} S(u^{\pm}, \nabla u^{\pm}) + V(u, \nabla u) dt \tag{17}$$

  - We approximate the time integrals with Gauss quadrature
  - We need a high order accurate approximation of the solution $\widetilde{u} = \widetilde{u}(x,t)$ in the space time grid cell $Q \times [t_n; t_{n+1}]$

Space Time Expansion II

- We start with a Taylor space time expansion of the approximative solution at $t = t_n$ and $x = x_B$.

$$\widetilde{u}(x,t) = \sum_{j=1}^{p} \left[(t - t_n)\partial_t + (x - x_B) \cdot \nabla \right]^j u \Big|_{(x_B, t_n)} \tag{18}$$

- We want that $\widetilde{u}(x, t = t_n) = u^n(x)$, thus the pure space derivatives are already available from the DG polynomial
- The mixed space-time and pure time derivatives are approximated using the so-called Cauchy-Kowalewskaya procedure:
  - Example: Burgers equation $u_t = -u\,u_x$

$$\begin{aligned} u_{tx} &= -u_x^2 - uu_{xx} \\ u_{tt} &= -u_t u_x - uu_{xt} \\ u_{tt} &= -(-uu_x)u_x - u(-u_x^2 - uu_{xx}) \\ &\ldots \end{aligned} \tag{19}$$

Space Time Expansion III

- The local time stepping feature
  - We drop global time levels t_n and introduce the local time level t_{n_i} for every grid cell Q_i
  - We can use the STE approach, just change integration limits to the grid cells local times

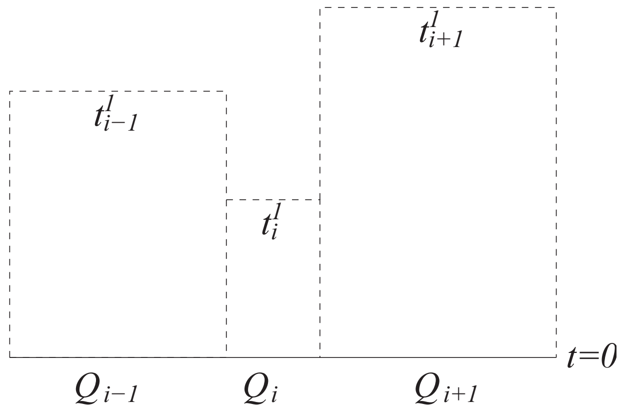
$$\left\langle u^{n+1}, \phi \right\rangle_{Q_I} = \langle u^n, \phi \rangle_{Q_i} + \int_{t_{n_i}}^{t_{n_i+1}} S(u^{\pm}, \nabla u^{\pm}) + V(u, \nabla u) dt \tag{20}$$

  - The RHS of the STE-DG formulation consists of 2 parts:
    - The space-time volume integral needs only local data from the own grid cell. Using the Taylor expansion, this part could be easily evaluated using the approximation $\widetilde{u}$ at the space-time Gauss points.
    - The space-time surface integral needs **more care**, as not only local data, but also data from the adjacent grid cells is needed for the numerical fluxes.

Local Time Stepping I

- To get a stable, high order accurate time consistent and conservative scheme, every grid cell has to satisfy the following **evolve condition**

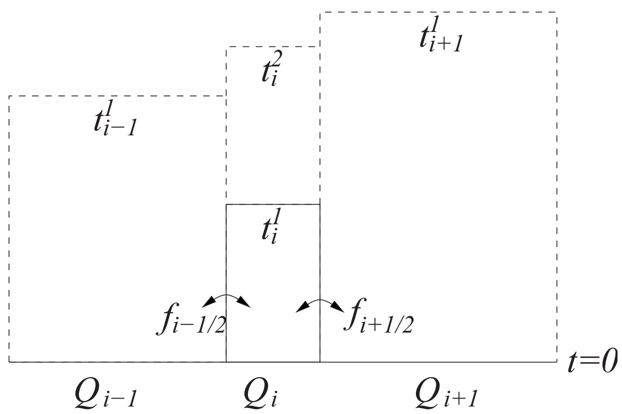
$$t^i_{n_i+1} \leq \min\{t^{i-1}_{n_{i-1}+1}, t^{i+1}_{n_{i+1}+1}\}$$



Local Time Stepping II

- To get a stable, high order accurate time consistent and conservative scheme, every grid cell has to satisfy the following **evolve condition**

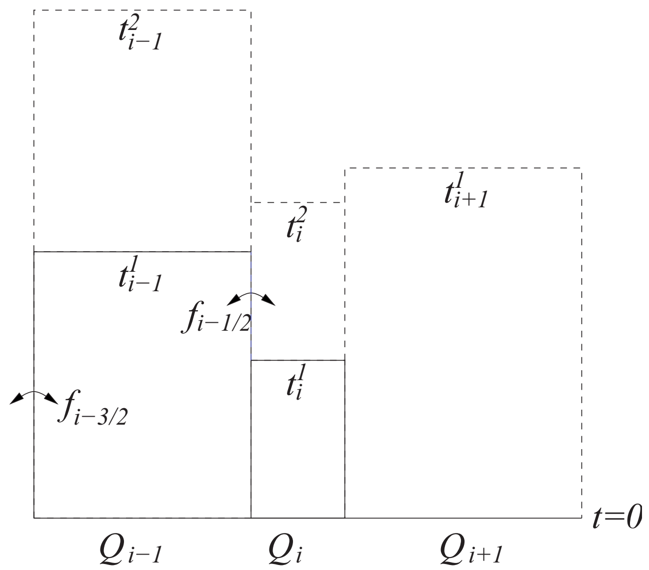
$$t^{i}_{n_i+1} \leq \min\{t^{i-1}_{n_{i-1}+1}, t^{i+1}_{n_{i+1}+1}\}$$



Local Time Stepping III

- To get a stable, high order accurate time consistent and conservative scheme, every grid cell has to satisfy the following **evolve condition**

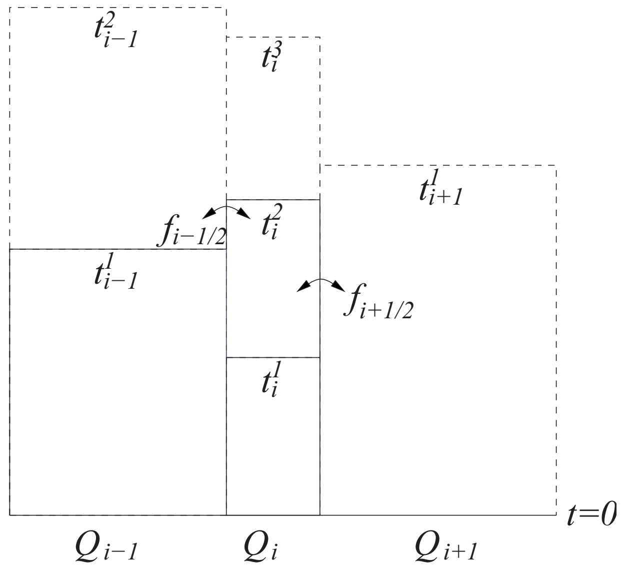
$$t^{i}_{n_i+1} \leq \min\{t^{i-1}_{n_{i-1}+1}, t^{i+1}_{n_{i+1}+1}\}$$



Local Time Stepping IV

- To get a stable, high order accurate time consistent and conservative scheme, every grid cell has to satisfy the following **evolve condition**

$$t^{i}_{n_i+1} \leq \min\{t^{i-1}_{n_{i-1}+1}, t^{i+1}_{n_{i+1}+1}\}$$



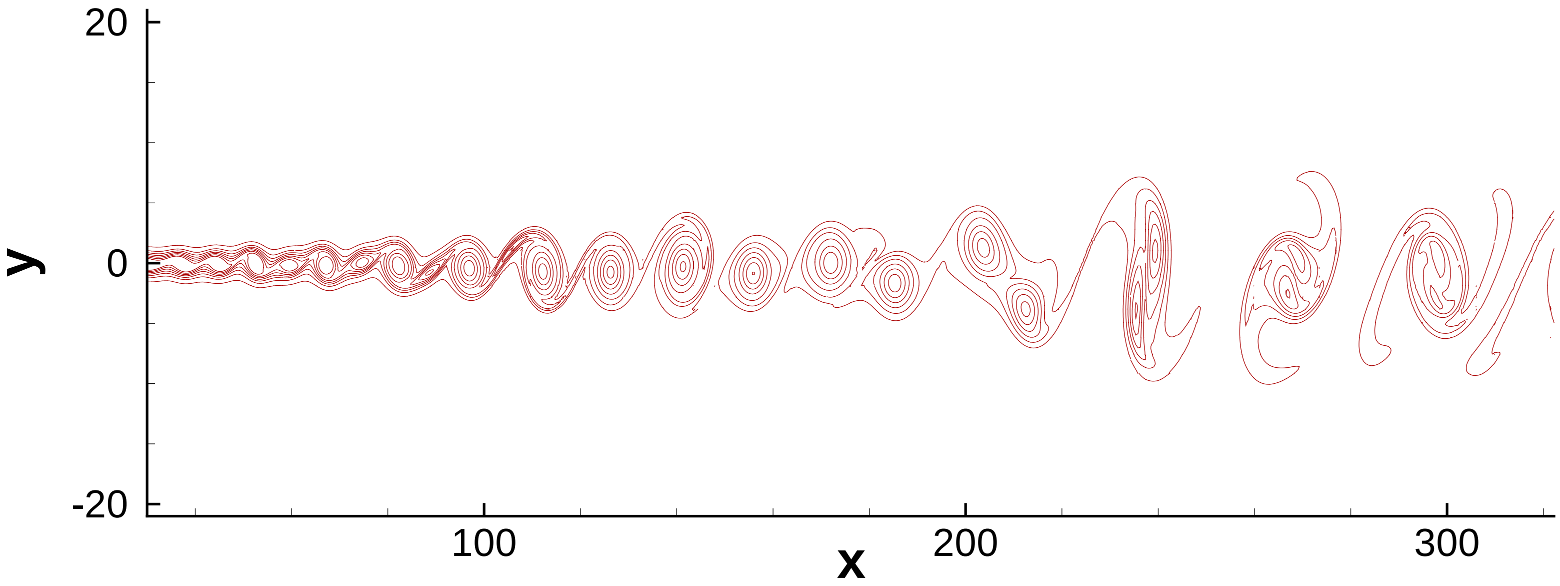
Local Time Stepping V

- Visualization of the local time stepping algorithm
  - 1D Euler equations
  - Irregular grid
  - As the problem is nonlinear, the local time steps depend on the solution!
  - Local time stepping space-time grid
- p-adaptation fully integrated in local time stepping algorithm
- p-adaptation STE-DG scheme fully parallelized and combined with dynamic load balancing
- first tests indicate excellent speed up and scale up efficiency for $\mathcal{O}(1000)$ processors
- more evaluations and applications are needed...

Result I

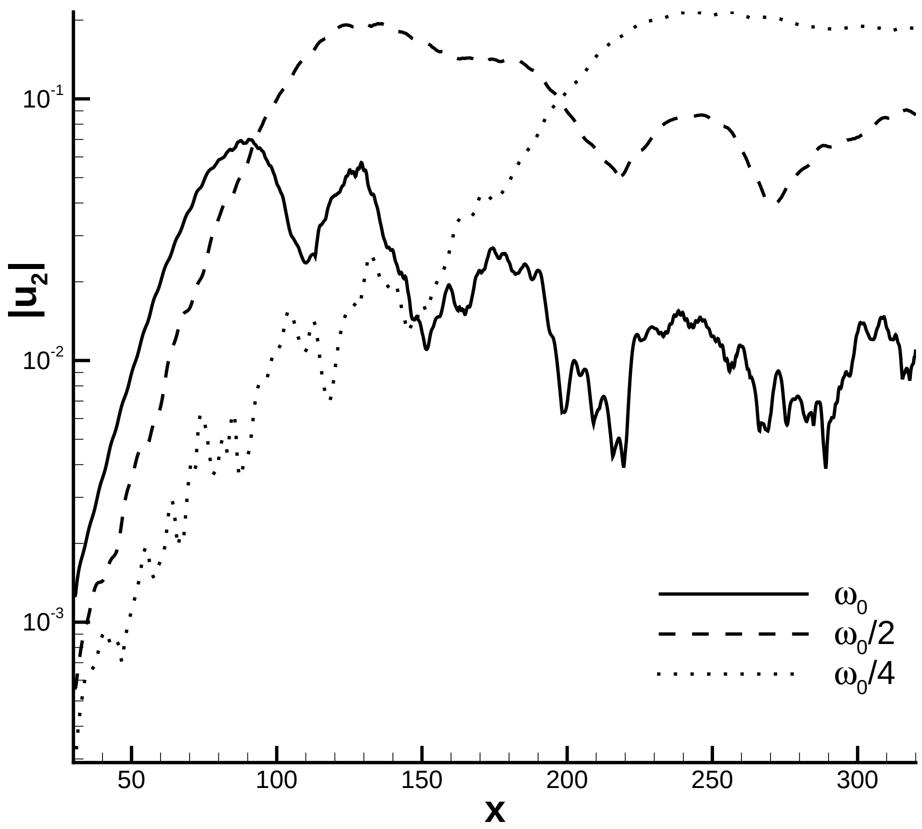
- Linear Stability Theory

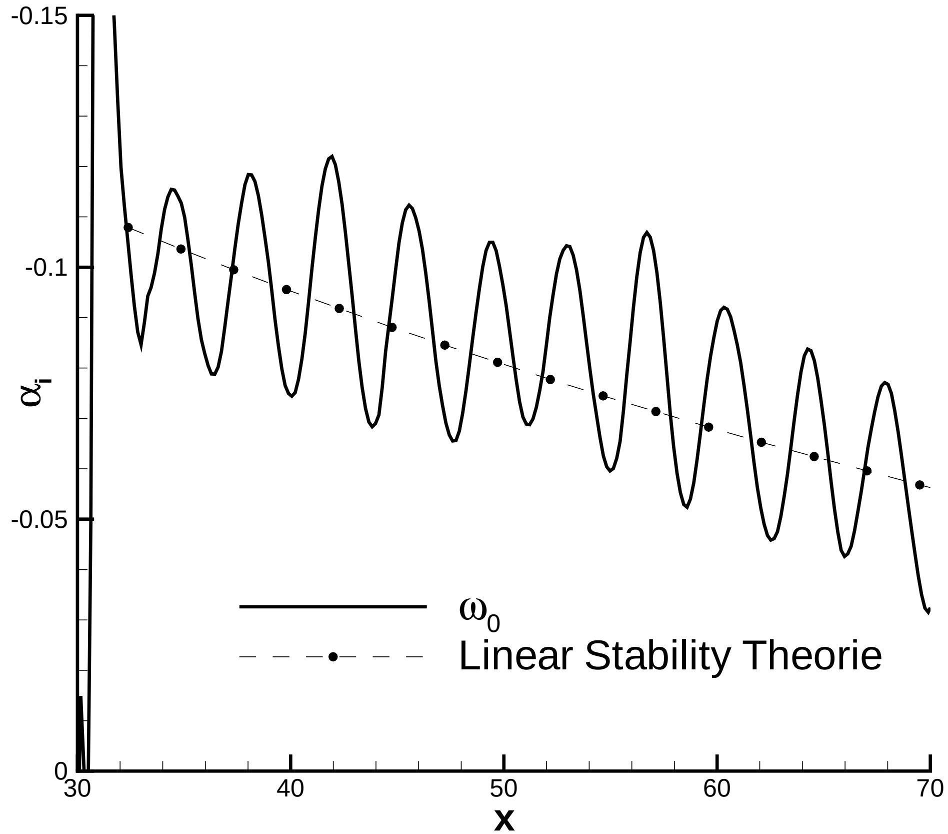
  - Shear layer ($M_1 = 0.5$, $M_2 = 0.25$ and $Re_1 = 500$)
  - 2D compressible Navier-Stokes equations
  - ≈ 180.000 DOF $p = 6$ STE-DG



Result I

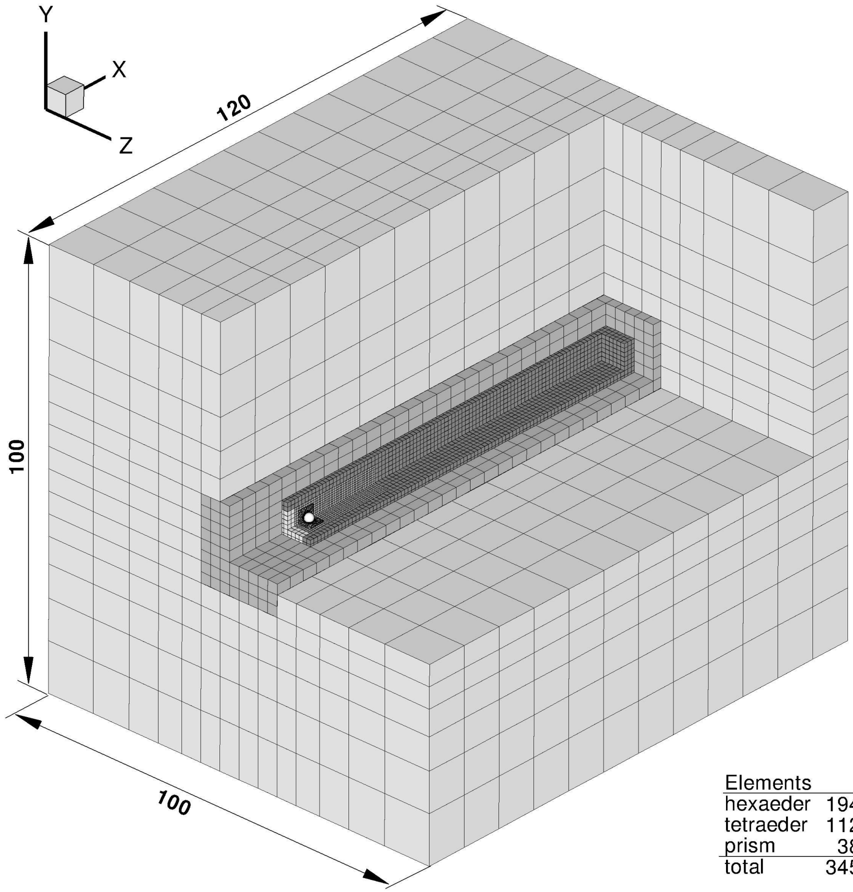
- Linear Stability Theory



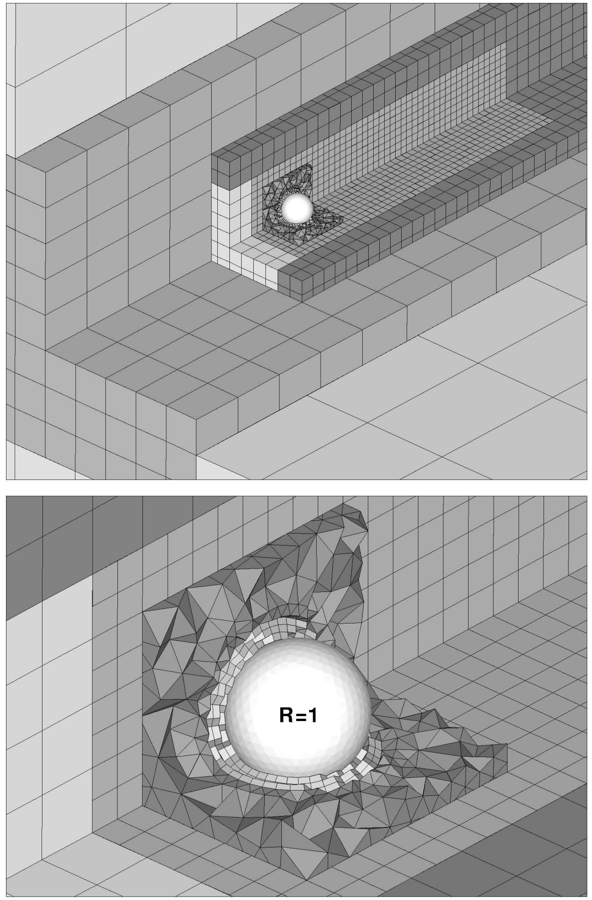


Result II

- Flow past a sphere ($M = 0.1$, $Re_D = 300$)



Elements	
hexaeder	19448
tetraeder	11211
prism	3876
total	34535



boundary layer $p = 5$, vortex street $p = 4$, far field $p = 1$ (≈ 1.2 Mio. DOF)

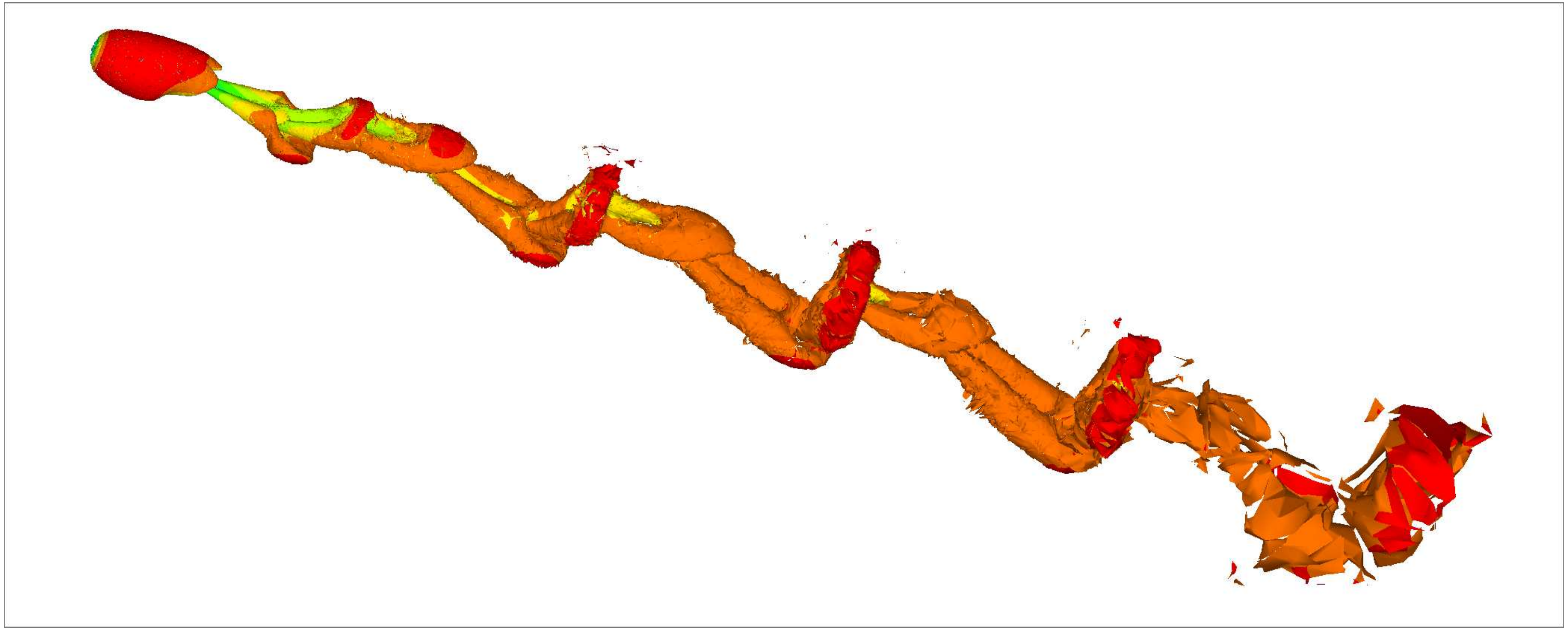
Result II

- Flow past a sphere ($M = 0.1$, $Re_D = 300$)
  - Drag, lifting coefficients and Strouhal number

	C_d	ΔC_d	C_l	ΔC_l	Str
	0.673	0.0031	−0.065	0.015	0.135
Tomboulides 1993	0.671	0.0028	–	–	0.136
Johnson&Patel 1999	0.656	0.0035	−0.069	0.016	0.137

Result II

- Flow past a sphere ($M = 0.1$, $Re_D = 300$)
  - Vortex detection using λ_2 criterion



(a) λ_2 iso surface

Outlook

- Hybrid unstructured 3D Code
- Explicit, arbitrary high order accurate in space and time, well suited for high performance computing
- Time accurate local time stepping
- p-adaptation in space and time
- Current Task: combine VMS-LES with STE-DG scheme

Parallelization I

- Scale up test, constant load per processor (150.000 DOF)

$\mathbf{n_P}$	1	8	64	512	2197
wallclock time(s)	803	816	818	834	851
efficiency (%)	100.0	98.5	98.2	96.4	94.5

- Speed up test: Shear layer (180.000 DOF)

$\mathbf{n_P}$	50	100	400
Nb DOF/proc	~ 3600	~ 1800	~ 900
efficiency (%)	100.0	101.0	98.1

- Blast Wave Problem with p-adaptation