Hardware-Oriented Numerics for PDEs

Solving Compressible Flow Problems by Isogeometric Analysis

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Acknowledgements

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Collaborators

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MOTOR

Multi-ObjecTive design Optimization of fluid eneRgy machines

Overview

1. From Numerical Analysis to Hardware-Oriented Numerics
2. Computational Building Blocks: Smart Fast Expression Templates
3. Application: Compressible flow solver
4. Isogeometric Analysis
5. Applications: Flow Problems, Meshing, and Optimization

Numerical Analysis: Past, Present, and Future(?)

Given a *problem* $p \in \mathcal{P}$:

1. Find a *method* $m \in \mathcal{M}$ that solves problem p

2. Find an *algorithm* $a \in \mathcal{A}$ that realizes method m

QoI: errors, rate of convergence, FLOP, stability, monotonicity, ...

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Given a *hardware* $h \in \mathcal{H}$:

3. Find an *implementation* $i \in \mathcal{I}$ that realizes algorithm a

QoI: FLOPS, memory bandwidth, parallel speed-up, ...

Numerical Analysis: Past, Present, and Future(?)

Given a *problem* $p \in \mathcal{P}$: $-\Delta u = f$ + bc's

1. Find a *method* $m \in \mathcal{M}$ that solves problem p
   continuous Galerkin P_1-FEM
2. Find an *algorithm* $a \in \mathcal{A}$ that realizes method m
   matrix-free CG solver with element-wise Gaussian quadrature

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   OpenMP parallelized SHMEM C++ code using Eigen library

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THE metric that matters: time to solution for prescribed accuracy

Hardware-Oriented Numerics

State of the art

Given a problem $p \in \mathcal{P}$ and a target hardware $h \in \mathcal{H}$:

1. Find an *optimal combination* $(m, a, i)_{p,h} \in \mathcal{M} \times \mathcal{A} \times \mathcal{I}$ that solves problem p on hardware h in shortest time with prescribed accuracy

Hardware-Oriented Numerics

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Given a problem $p \in \mathcal{P}$ and a set of target hardware $\{h_1, h_2, \dots\} \subset \mathcal{H}$:

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Next step

2. Develop a strategy that automatically inspects the available hardware and chooses the optimal combinations $(m, a, i)_{p,h_k}$

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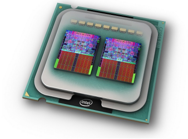
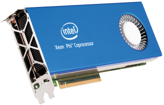
Future vision

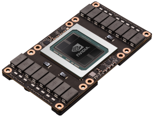
3. Automatically determine and schedule optimal combinations $(m, a, i)_{p_j,h_k} \in \mathcal{M} \times \mathcal{A} \times \mathcal{I}$ for multi-physics problems $\{p_1, p_2, \dots\} \subset \mathcal{P}$ and target hardware $\{h_1, h_2, \dots\} \subset \mathcal{H}$

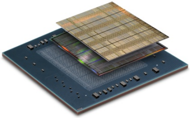
HPC hardware

Current and (most probably) future HPC hardware is diversified:









multi-core CPUs many-core MICs and GPUs FPGAs

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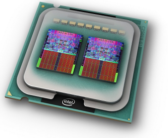
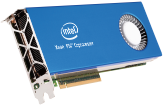
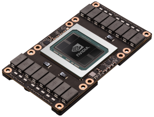


multi-core CPUs





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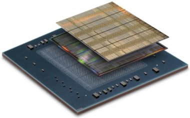

FPGAs

There are good reasons (performance-per-watt, low-latency) to believe that the future of HPC lies in heterogeneous and hybrid technologies:

CPUs + accelerators

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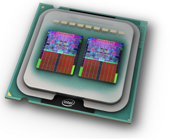

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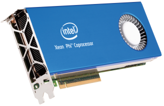

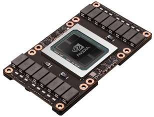

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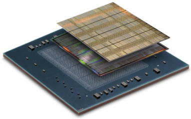

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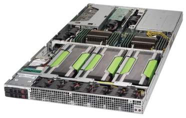

CPUs + accelerators

Stand-alone Xeon Phi

HPC hardware

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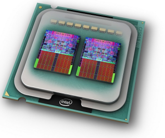

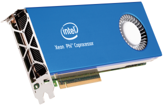

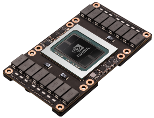

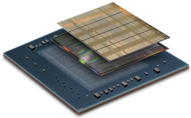

multi-core CPUs | many-core MICs and GPUs | FPGAs

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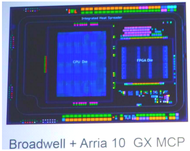


CPUs + accelerators | Stand-alone Xeon Phi | Hybrid CPU/FPGA

HPC hardware and beyond

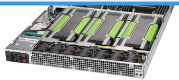
Quantum Computing

Strong effort in the Netherlands to establish quantum computers and algorithms as key technology in future scientific computing

QuSoft QUTech

Application in PDE-constrained optimization

- $\exists$ QA to estimate $x^\top Mx$ s.t. $Ax = b$ in poly$(\log N, \log(1/\epsilon))$
- best classical algorithm requires $\mathcal{O}(N\sqrt{\kappa})$



CPUs + accelerators

Stand-alone Xeon Phi

Hybrid CPU/FPGA

Question 1

Can we come up with a **unified programming approach** to exploit the performance of the different hardware architectures automatically with minimal effort for code development and maintenance?

Computational building blocks

- Highly optimized dense and sparse linear algebra libraries

$$y \leftarrow \alpha * x + y, \quad y \leftarrow A^{-1} * x$$

BLAS/LAPACK implementation of $y \leftarrow A^{-1}(x - y)$

```
call xSCAL(n, -1.0, y, 1)
call xAXPY(n,  1.0, x, 1, y, 1)
call xGESV(n, 1, A, n, IPIV, y, 1, INFO)
```

Here: 3 function calls, 5× fetching data, 3× storing data.

Ideal: no call (inlining!), 3× fetching data, 1× storing data.

And it's the memory transfer that is the bottleneck!

Computational building blocks

- Highly optimized dense and sparse linear algebra libraries

$$y \leftarrow \alpha * x + y, \quad y \leftarrow A^{-1} * x$$

- Expression template libraries (ETLs)

$$y \leftarrow A * ((m. * m)./(\rho) + p)$$

Note: against common belief, the use of ETLs does not automagically lead to high-performance C++ code

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- *Smart and fast expression template libraries* which combine classical ETL concepts with vector intrinsics, node-level parallelization, cache-size/architecture optimized compute kernels

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- *Smart and fast expression template libraries* which combine classical ETL concepts with vector intrinsics, node-level parallelization, cache-size/architecture optimized compute kernels
- *Just-in-time compilation* ('reconfigurable computing')

SFET concept

Code that you write[1]

```
vex::vector<float> x,y,z;   z = x * y;
```

OpenCL compute kernel generated by VexCL

```
kernel void vexcl_kernel(...) {
  for(size_t idx = get_global_id(0);
             idx < n;
             idx += get_global_size(0)) {
    prm_1[idx] = prm_2[idx] * prm_3[idx]; }}
```

[1] https://github.com/ddemidov/vexcl

SFET concept

Code that you write[1]

```
vex::vector<float> x,y,z;    z = x * y;
```

CUDA compute kernel generated by VexCL

```
extern "C" __global__ void vexcl_kernel(...) {
  for(size_t idx = blockDim.x * blockIdx.x
                 + threadIdx.x,
             grid_size = blockDim.x * gridDim.x;
             idx < n;
             idx += grid_size) {
    prm_1[idx] = prm_2[idx] * prm_3[idx]; }}
```

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SFET concept

Code that you write[1]

```
vex::vector<float> x,y,z;    z = x * y;
```

MaxJ compute kernel to be generated by VexCL (D.Pouw)

```
class vexcl_kernel extends Kernel {
  public vexcl_kernel(...) {
    DFEVar x = io.input("x", dfeFloat(8, 24));
    DFEVar y = io.input("y", dfeFloat(8, 24));

    DFEVar result = x * y;
    io.output("z", result, dfeFloat(8, 24)); }}
```

[1] https://github.com/ddemidov/vexcl

Compressible Euler equations

Divergence form

$$\partial_t U + \nabla \cdot \mathbf{F}(U) = 0$$

Quasi-linear form

$$\partial_t U + \mathbf{A}(U) \cdot \nabla U = 0$$

Conservative[a] **variables**, inviscid **fluxes**, flux-Jacobian **matrices**

$$U = \begin{bmatrix} \rho \\ \rho \mathbf{v} \\ \rho E \end{bmatrix}, \qquad \mathbf{F} = \begin{bmatrix} \rho \mathbf{v} \\ \rho \mathbf{v} \otimes \mathbf{v} + \mathcal{I} p \\ \mathbf{v}(\rho E + p) \end{bmatrix}, \qquad \mathbf{A} = \frac{\partial \mathbf{F}}{\partial U}$$

Equation of state (here for an ideal gas)

$$p = (\gamma - 1)\left(\rho E - \frac{1}{2}\rho \|\mathbf{v}\|^2\right), \quad \gamma = C_p / C_v$$

[a] Similar formulations exist for primitive and entropy variables

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$$U = \begin{bmatrix} u_1 \\ \vdots \\ u_{d+2} \end{bmatrix}, \qquad \mathbf{F} = \begin{bmatrix} f_1^1 & \cdots & f_1^d \\ \vdots & \ddots & \vdots \\ f_{d+2}^1 & \cdots & f_{d+2}^d \end{bmatrix}, \qquad \mathbf{A} = \frac{\partial \mathbf{F}}{\partial U}$$

Notation

$$\mathbf{f}_k = \left[f_k^1, \ldots, f_k^d \right], \qquad \mathbf{f}^k = \begin{bmatrix} f_1^k \\ \vdots \\ f_{d+2}^k \end{bmatrix}$$

[a]Similar formulations exist for primitive and entropy variables

Fluid Dynamics Building Blocks[2]

High-level

SFET's for conservative/primitive variables, EOS, inviscid/viscous fluxes, flux Jacobians, and Riemann solvers

Low-level

Unified wrapper function API to core functionality of ETL's: make_temp, tag, tie, +, -, *, /, abs, sqrt, ...

Armadillo | ArrayFire | Blaze | Blitz++ | Eigen | IT++ | MTL4 | uBLAS | VexCL | ViennaCL | ...

[2] https://gitlab.com/mmoelle1/FDBB.git

FDBB at work

Implementation of $\|\mathbf{v}\|^2$

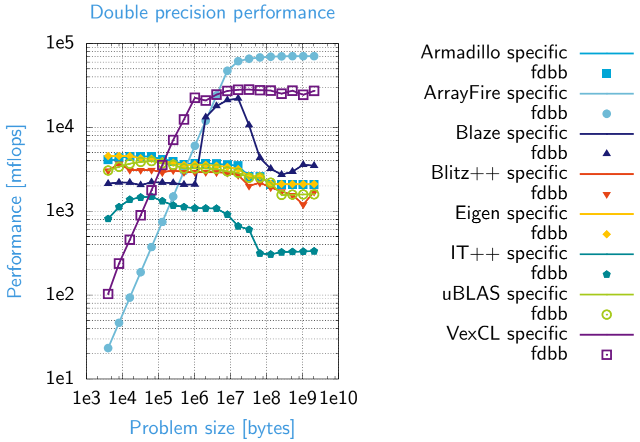
```
// EOS for ideal gas (gamma=1.4)
typedef fdbb::fdbbEOSidealGas<T> eos;

// Conservative variables in 3d
typedef fdbb::fdbbVariables<eos,3,
        fdbb::EnumVar::conservative> var;

// VexCL backend
vex::vector<T> u1,u2,u3,u4,u5,v;

// Generic implementation
v = var::v_mag2(u1,u2,u3,u4,u5);
```

FDBB μ-benchmark

- All tests were run under CentOS Linux 6.7, GCC 5.3.0, nvcc 7.5.17 with thread pinning (`likwid-pin -c N:0-15 benchmark`)
- CPU benchmarks
  - 2x Intel E5-2670 (16 cores), 2.60GHz, 20MB Cache, 64GB RAM
  - ETL's: Armadillo, Blaze, Blitz++, Eigen, IT++, uBLAS
- GPU benchmarks
  - 1x NVIDIA Tesla K20Xm, ECC off, 6GB (DriVer: 352.93)
  - ETL's: ArrayFire and VexCL with CUDA backend enabled

FDBB μ-benchmark

$$y \leftarrow (m_x . * m_x + m_y . * m_y + m_z . * m_z)./(\rho . * \rho) \qquad \text{7 flop}$$



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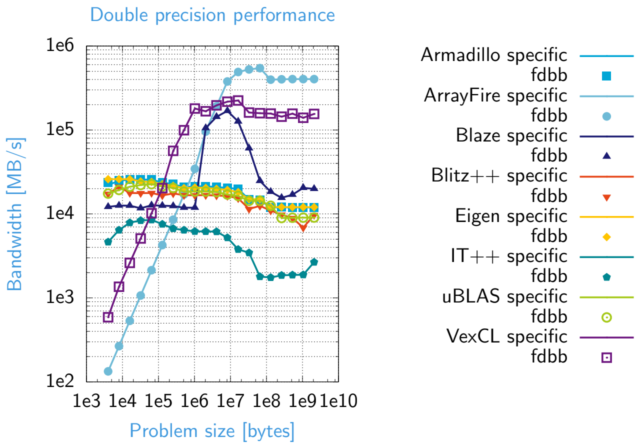

Question 2

Given we have a highly tuned SFET library (and FDBB), how can we design a **compressible flow solver** based on SpMV and at the same time flexible enough for practical applications?

Compressible Euler equations

Galerkin ansatz ("find solution U s.t. for all W")

$$\int_\Omega W\partial_t U - \nabla W \cdot \mathbf{F}(U)\,\mathrm{d}\Omega + \int_\Gamma W F^b(U,\cdot)\,\mathrm{d}s = 0$$

with boundary fluxes

$$F^b = \begin{cases} [0, pn_1, pn_2, pn_3, 0]^\top & \text{at solid walls} \\ \frac{1}{2}(F_n(U_-) + F_n(U_+)) - \frac{1}{2}|A_n(\mathrm{Roe}(U_-, U_+))| & \text{otherwise} \end{cases}$$

[3] C.A.J. Fletcher, CMAME 37 (1983) 225–244.

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Fletcher's group formulation[3]

$$U_h = \sum_A (\mathcal{I} \otimes \varphi_A(\mathbf{x})) U_A(t), \quad \mathbf{F}_h = \sum_A (\mathcal{I} \otimes \varphi_A(\mathbf{x})) \mathbf{F}_A(t), \quad \mathbf{F}_A = \mathbf{F}(U_A)$$

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Compressible Euler equations

Semi-discretized problem

$$\begin{bmatrix} M & & \\ & \ddots & \\ & & M \end{bmatrix} \begin{bmatrix} \dot{u}_1 \\ \vdots \\ \dot{u}_{d+2} \end{bmatrix} + \begin{bmatrix} \mathbf{C} & & \\ & \ddots & \\ & & \mathbf{C} \end{bmatrix} \begin{bmatrix} \mathbf{f}_1^\top \\ \vdots \\ \mathbf{f}_{d+2}^\top \end{bmatrix} + \begin{bmatrix} \mathbf{S} & & \\ & \ddots & \\ & & \mathbf{S} \end{bmatrix} \begin{bmatrix} \mathbf{f}_1^{b^\top} \\ \vdots \\ \mathbf{f}_{d+2}^{b^\top} \end{bmatrix} = 0$$

Read the above as

$$\mathbf{C}\mathbf{f}_k^\top = \left[C^1, \dots, C^d\right] \begin{bmatrix} f_k^1 \\ \vdots \\ f_k^d \end{bmatrix} = \sum_{l=1}^{d} C^k f_k^l \qquad \text{for } k = 1, \dots, d+2$$

and the same for $\mathbf{S}\mathbf{f}_k^{b^\top}$

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Constant coefficient matrices

$$M = \left[\int_\Omega \varphi_A \varphi_B \, \mathrm{d}\Omega \right] \quad \mathbf{C} = \left[- \int_\Omega \nabla \varphi_A \varphi_B \, \mathrm{d}\Omega \right] \quad \mathbf{S} = \left[\int_\Gamma \varphi_A \varphi_B \mathbf{n} \, \mathrm{d}s \right]$$

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whereby

$$- \int_\Omega \nabla \varphi_A \varphi_B \, \mathrm{d}\Omega = \int_\Omega \varphi_A \nabla \varphi_B \, \mathrm{d}\Omega + \int_\Gamma \varphi_A \varphi_B \mathbf{n} \, \mathrm{d}s \quad \Rightarrow \quad \mathbf{C} + \mathbf{C}^\top = \mathbf{S}$$

Stabilization by algebraic flux correction

$$(\mathcal{I} \otimes m_A)\dot{U}_A + \sum_B \left(\mathbf{c}_{AB} \cdot \mathbf{F}_B + \mathbf{s}_{AB} \cdot \mathbf{F}_B^b\right) + \sum_{B \in \mathcal{J}_A} D_{AB}(U_B - U_A) = \sum_{B \in \mathcal{J}_A} \alpha_{AB} \mathcal{F}_{AB}$$

1. Perform row-sum mass lumping to decouple the degrees of freedom
2. Add discrete artificial dissipation to prevent spurious oscillations
3. Decompose anti-diffusion into fluxes and apply a limited correction

Details:

- Kuzmin, M., Gurris, AFC II. Compressible Flow Problems. In: Flux-Corrected Transport, Springer, 2012

Stabilization by algebraic flux correction

$$(\mathcal{I} \otimes m_A)\dot{U}_A + \sum_B \left(\mathbf{c}_{AB} \cdot \mathbf{F}_B + \mathbf{s}_{AB} \cdot \mathbf{F}_B^b\right) + \sum_{B \in \mathcal{J}_A} D_{AB}(U_B - U_A) = \sum_{B \in \mathcal{J}_A} \alpha_{AB} \mathcal{F}_{AB}$$

Compute kernels

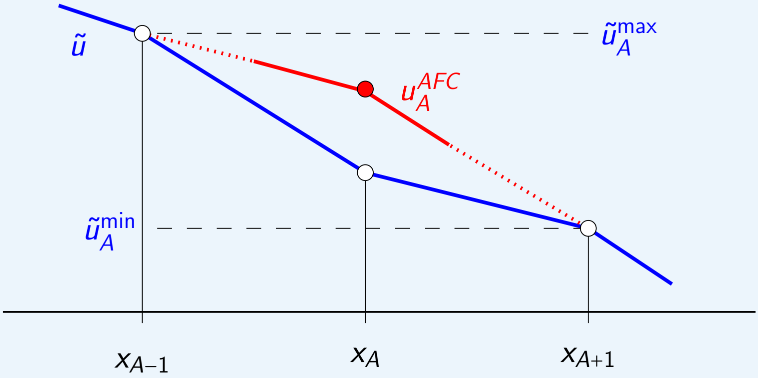
- block-VV and block-SpMV
- edge-loops over non-zero entries of sparsity graph

$$\mathcal{I}_A := \{B \,:\, \mathrm{supp}\varphi_A \cap \mathrm{supp}\varphi_B \neq \emptyset\}, \quad \mathcal{J}_A := \mathcal{I}_A \setminus \{A\}$$

  - symmetric operators D_{AB} and α_{AB}
  - skew-symmetric fluxes $U_B - U_A$ and $\mathcal{F}_{AB}$

$\Rightarrow$ can be expressed as block-SpMV

Illustration of Zalesak's flux limiter[4]



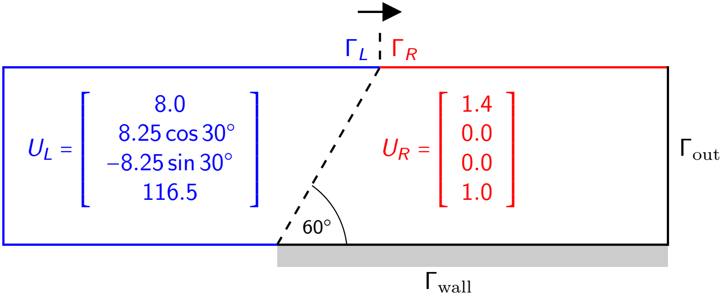
- Mass-lumped low-order predictor yields nodal bounds $\tilde{u}_A^{\overset{max}{min}}$
- AFC-corrected solution is allowed to vary within the bounds

[4] S. Zalesak, JCP 1979, 31(3), 335–362

Double Mach reflection[5]

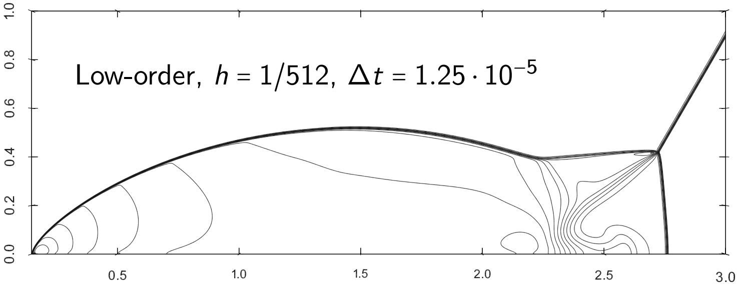
Test: Roe-linearization + FCT, structured mesh, Q_1 finite elements

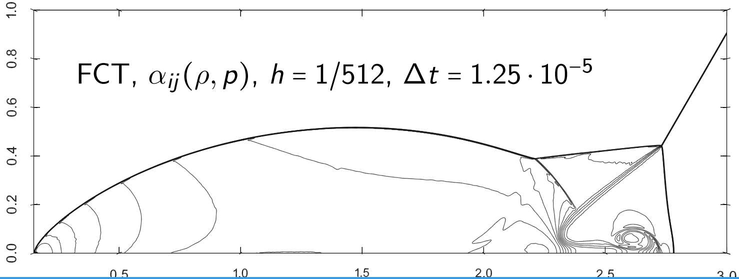
$T = 0.2$, Crank Nicolson time stepping ($\theta = 0.5$)



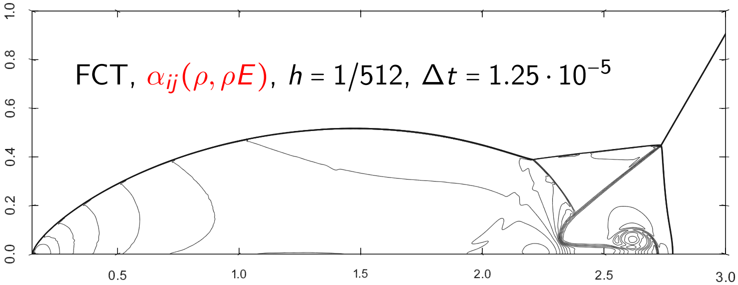
[5] P.R. Woodward, P. Colella, JCP 54, 115 (1984), 115–173.

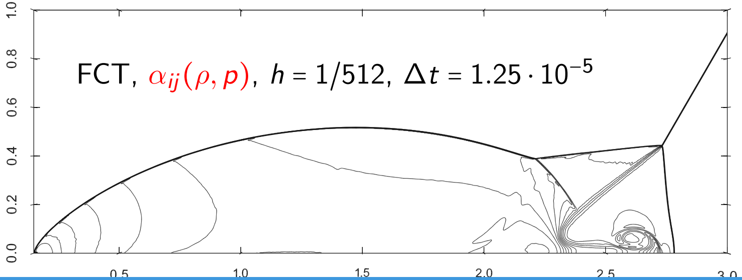
Double Mach reflection





Double Mach reflection





Question 3

The presented approach is applicable to unstructured meshes and general FE spaces except for AFC which is limited to P_1 and Q_1!

It there a way to extend AFC to **higher-order approximations**?

Polynomial spaces

Definition

The space of polynomials of degree p over the interval $[a,b]$ is

$$\Pi^p([a,b]) := \{q(x) \in \mathcal{C}^\infty([a,b]) \,:\, q(x) = \sum_{i=0}^{p} c_i x^i,\, c_i \in \mathbb{R}\}$$

Example: $\Pi^2([0,1])$

- Canonical basis

$$\mathcal{B} = \{1, x, x^2\}$$

- Polynomials

$$q(x) = c_0 + c_1 x + c_2 x^2$$

Spline space

Definition

Let $\mathcal{P} = \{a = x_1 < \cdots < x_{p+1} = b\}$ be a partition of the interval Ω_0 and $\mathcal{M} = \{1 \leq m_i \leq p+1\}$ a set of positive integers. The polynomial spline of degree p is defined as $s : \Omega_0 \mapsto \mathbb{R}$ if

$$s\big|_{[x_i, x_{i+1}]} \in \Pi^p([x_i, x_{i+1}]), \qquad i = 1, \ldots, k$$

$$\frac{d^j}{dx^j} s_{i-1}(x_i) = \frac{d^j}{dx^j} s_i(x_i), \qquad \begin{array}{l} i = 2, \ldots, k, \\ j = 0, \ldots, p - m_i \end{array}$$

Polynomial splines of degree p form the spline space $\mathcal{S}(\Omega_0, p, \mathcal{M}, \mathcal{P})$.

Knot vectors

Definition

A knot vector is a sequence of non-decreasing values $\xi_i \in [a, b] \subset \mathbb{R}$ in the parameter space $\Omega_0 = [a, b]$

$$\Xi = (\xi_1, \xi_2, \ldots, \xi_{n+p+1})$$

where

- p is the polynomial order of the B-splines
- n is the number of B-spline functions
- ξ_i is the i-th knot with knot index i

Knots ξ_i can have multiplicity $1 \leq m_i \leq p + 1$. The knot vector is called open if the first and last knot have multiplicity $p + 1$.

B-spline basis functions

Cox-de Boor recursion formula

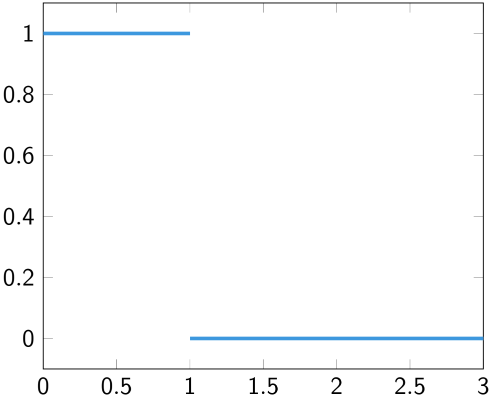
$p = 0$

$$N_{i,0}(\xi) = \begin{cases} 1 & \text{if } \xi_i \leq \xi < \xi_{i+1} \\ 0 & \text{otherwise} \end{cases}$$

$p > 0$

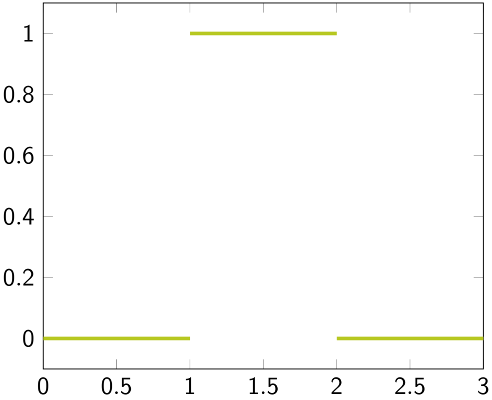
$$N_{i,p}(\xi) = \frac{\xi - \xi_i}{\xi_{i+p} - \xi_i} N_{i,p-1}(\xi) + \frac{\xi_{i+p+1} - \xi}{\xi_{i+p+1} - \xi_{i+1}} N_{i+1,p-1}(\xi)$$

B-spline basis functions



Constant basis functions corresponding to $\Xi = \{0, 0, 0, 1, 2, 3, 3, 3\}$

B-spline basis functions



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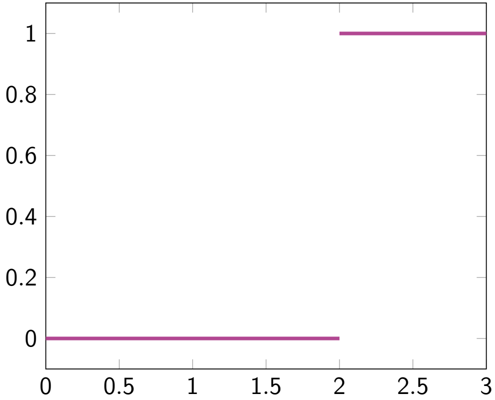

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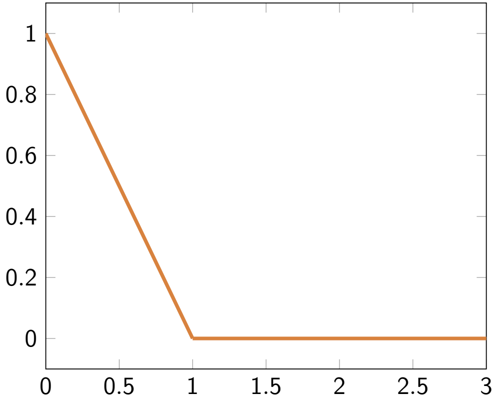
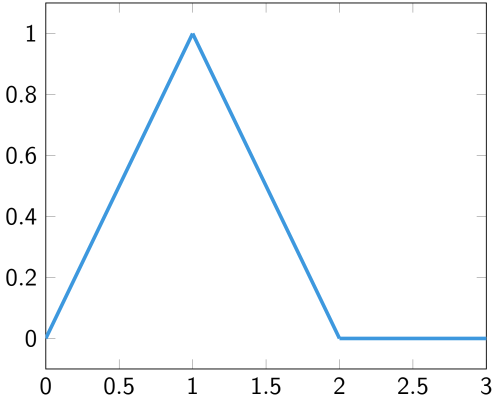


Linear basis functions corresponding to $\Xi = \{0, 0, 0, 1, 2, 3, 3, 3\}$

B-spline basis functions



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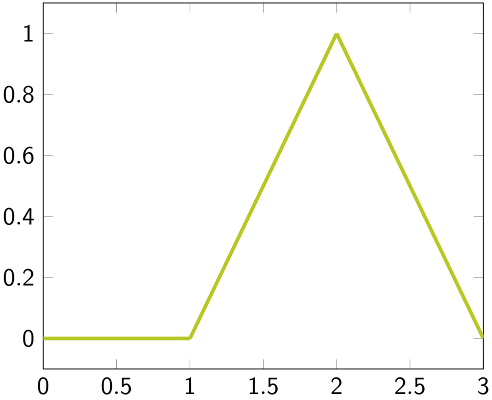

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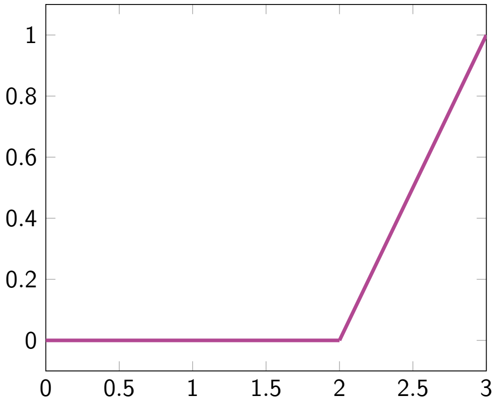

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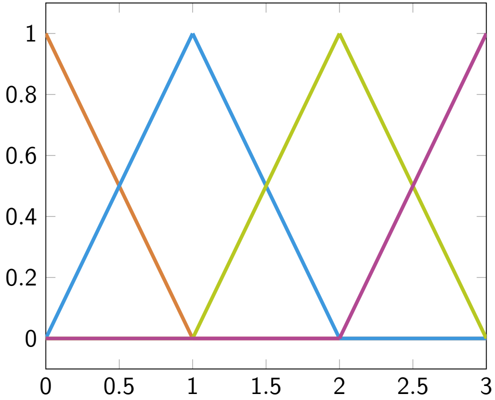

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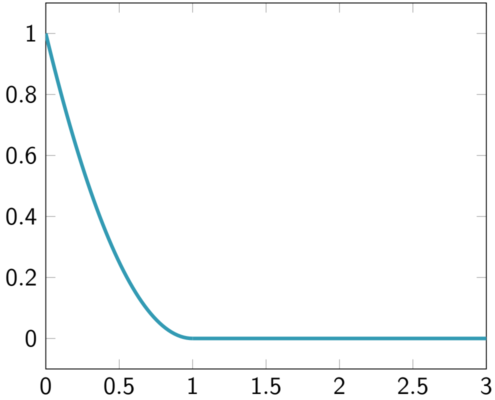
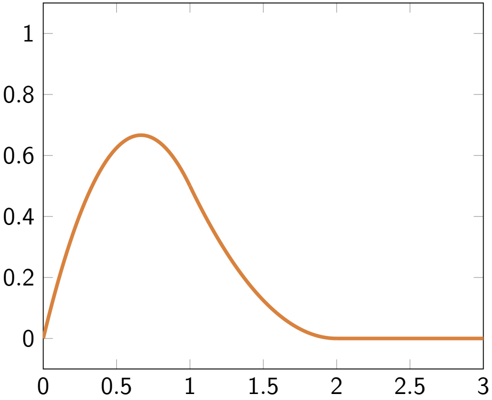


Quadratic basis functions corresponding to $\Xi = \{0, 0, 0, 1, 2, 3, 3, 3\}$

B-spline basis functions



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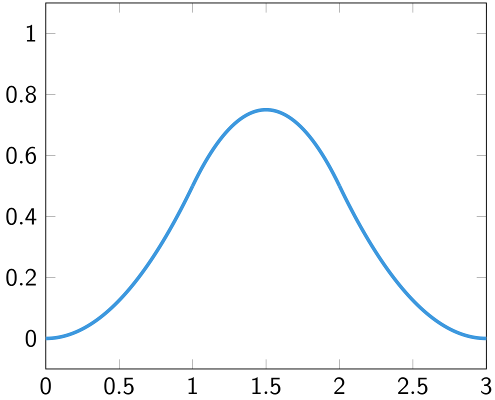

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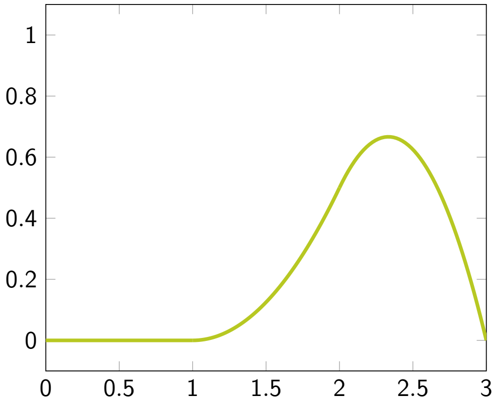

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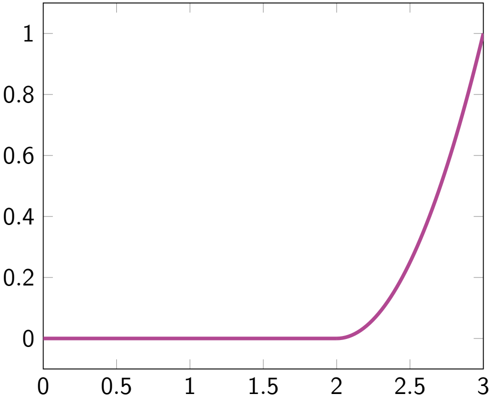

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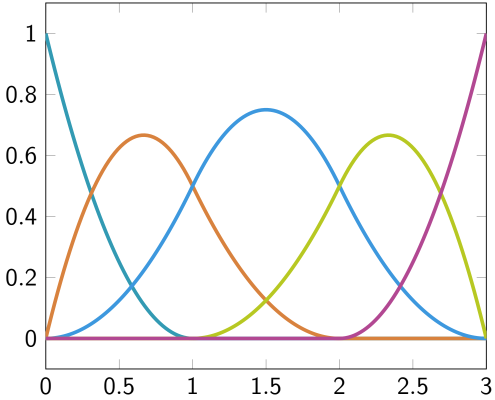
B-spline basis functions



Quadratic basis functions corresponding to $\Xi = \{0, 0, 0, 1, 2, 3, 3, 3\}$

Properties of B-spline basis functions

Compact support

$$\text{supp } N_{i,p}(\xi) = [\xi_i, \xi_{i+p+1}), \quad i = 1, \dots, n$$

- System matrices are sparse like in the standard FEM
- Support grows with the polynomial order so that system matrices have a slightly broader stencil due to the coupling of degrees of freedom over multiple element layers (good for HPC)

Properties of B-spline basis functions

Compact support

$$\text{supp } N_{i,p}(\xi) = [\xi_i, \xi_{i+p+1}), \quad i = 1, \ldots, n$$

Strict positiveness

$$N_{i,p}(\xi) > 0 \quad \text{for } \xi \in (\xi_i, \xi_{i+p+1}), \quad i = 1, \ldots, n$$

- Consistent mass matrix has no negative off-diagonal entries
- Lumped mass matrix is not singular (no zero diagonal entries)

Properties of B-spline basis functions

Compact support

$$\text{supp } N_{i,p}(\xi) = [\xi_i, \xi_{i+p+1}), \quad i = 1, \ldots, n$$

Strict positiveness

$$N_{i,p}(\xi) > 0 \quad \text{for } \xi \in (\xi_i, \xi_{i+p+1}), \quad i = 1, \ldots, n$$

Partition of unity

$$\sum_{i=1}^{n} N_{i,p}(\xi) = 1 \quad \text{for all } \xi \in [a, b]$$

Properties of B-spline basis functions

Derivatives

Derivative is a B-spline of order $p-1$

$$\frac{d}{d\xi}N_{i,p}(\xi) = \frac{p}{\xi_{i+p}-\xi_i}N_{i,p-1}(\xi) - \frac{p}{\xi_{i+p+1}-\xi_{i+1}}N_{i+1,p-1}(\xi)$$

Expression for k^{th} derivative

$$\frac{d^k}{d^k\xi}N_{i,p}(\xi) = \frac{p!}{(p-k)!}\sum_{j=0}^{k}\alpha_{k,j}N_{i+j,p-k}(\xi)$$

with recursively defined coefficients $\alpha_{k,j}$[a]

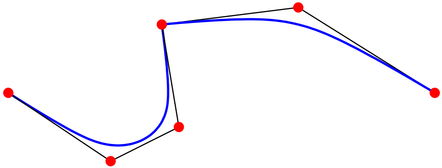
[a] L. Piegl, W. Tiller. The NURBS book (1997).

Spline curves

Geometric mapping $\mathbf{G} : \Omega_0 \mapsto \Omega_h \simeq \Omega$

$$\mathbf{G}(\xi) = \sum_{i=1}^{n} N_{i,p}(\xi)\mathbf{B}_i$$

set of control points $\mathbf{B}_i \in \mathbb{R}^d, d \geq 1$

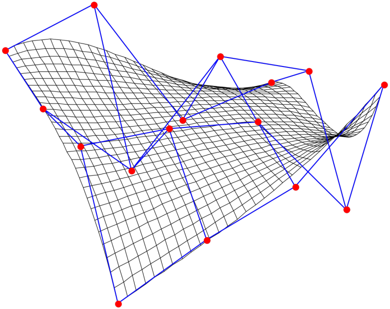


- C^{p-m_i} continuous curve (m_i is the multiplicity of knot ξ_i)
- Convex hull property
- Variation diminishing property
- Knot insertion (h-adaptivity), order elevation (p-adaptivity) preserve shape of geometry

Spline surfaces

Geometric mapping $\mathbf{G}: \Omega_0 \mapsto \Omega_h \simeq \Omega$

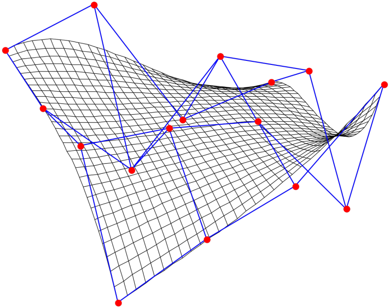
$$\mathbf{G}(\xi,\eta) = \sum_{i=1}^{n}\sum_{j=1}^{m} N_{i,p}(\xi)N_{j,q}(\eta)\mathbf{B}_{i,j} \qquad \mathbf{B}_{i,j} \in \mathbb{R}^d, d \geq 2$$



Spline surfaces

Geometric mapping $\mathbf{G} : \Omega_0 \mapsto \Omega_h \simeq \Omega$

$$\mathbf{G}(\xi) = \sum_{\mathbf{A}} \hat{\varphi}_{\mathbf{A}}(\xi)\mathbf{B}_{\mathbf{A}} \qquad \mathbf{B}_{\mathbf{A}} \in \mathbb{R}^d, d \geq 2, \text{ multi-index } \mathbf{A}$$



- Computational 'mesh' is a multi-variate parameterization of Ω_h. It can be canonically generated from the geometry by knot insertion and/or order elevation $(\hat{\varphi}_{\mathbf{A}}, \mathbf{B}_{\mathbf{A}}) \to (\tilde{\varphi}_{\mathbf{A}}, \tilde{\mathbf{B}}_{\mathbf{A}})$

Marriage of geometry and discretization

Geometric mapping

$$\mathbf{G}(\boldsymbol{\xi}) = \sum_{\mathbf{A}} \hat{\varphi}_{\mathbf{A}}(\boldsymbol{\xi}) \mathbf{B}_{\mathbf{A}} \qquad \text{'push-forward'} \ \mathbf{G} : \Omega_0 \mapsto \Omega_h$$

Ansatz space

$$V_h = \text{span}\{\varphi_{\mathbf{A}}(\mathbf{x}) = \tilde{\varphi}_{\mathbf{A}} \circ \mathbf{G}^{-1}(\mathbf{x})\} \qquad \text{'pull-back'} \ \mathbf{G}^{-1} : \Omega_h \mapsto \Omega_0$$

Question 4

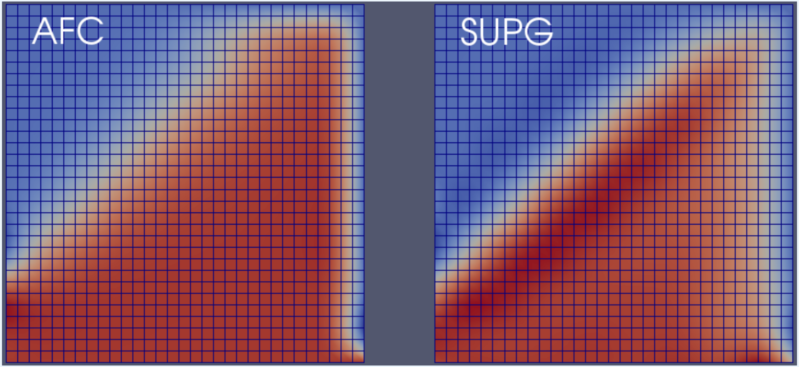
Bézier extraction is commonly promoted as 'the' way to integrate isogeometric analysis into classical finite element codes. But doesn't this contradict the concept of hardware-oriented numerics?

Our research is based on genuine IgA tools:

- C++ library G+SMO developed at JKU/RICAM, Linz
- Python library Nutils (Numerical Utilities) by Evalf Computing, Delft

Application: Convection-diffusion equation

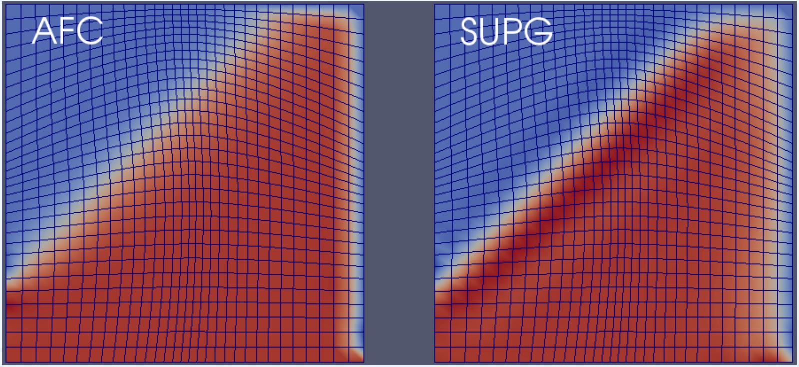
Convection skew to the mesh



Quadratic bi-variate B-spline basis functions.

Application: Convection-diffusion equation

Convection skew to the mesh



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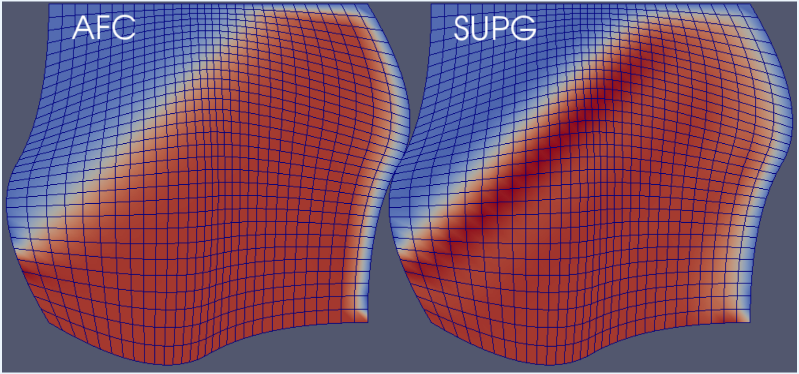
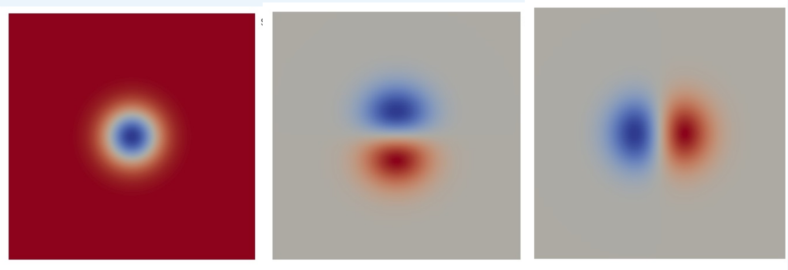


Quadratic bi-variate B-spline basis functions.

Application: Compressible Euler equations

Convection of isentropic vortex[6]



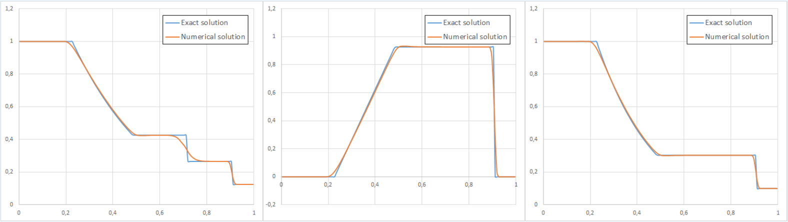
ρ $\qquad$ v_x $\qquad$ v_y

Quadratic bi-variate B-spline basis functions.

[6] H-C. Yee, N. Sandham, M. Djomehri, JCP 150 (1999) 199-238.

Application: Compressible Euler equations

Sod's shock tube problem[7]



ρ v_x p

Quadratic bi-variate B-spline basis functions.

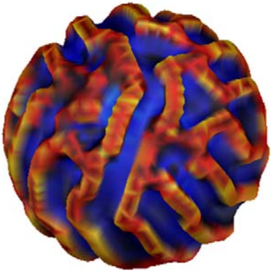
[7] G.A. Sod, JCP 27 (1978) 1–31.

Application: IgA on evolving manifolds

Gray-Scott reaction-diffusion model

$$u_t + u(\ln\sqrt{g_t})_t - d_1\Delta u = F(1-u) - uv^2$$
$$v_t + v(\ln\sqrt{g_t})_t - d_2\Delta v = -(F+H)v + uv^2$$
$$\mathbf{s} = Kv\mathbf{n}$$

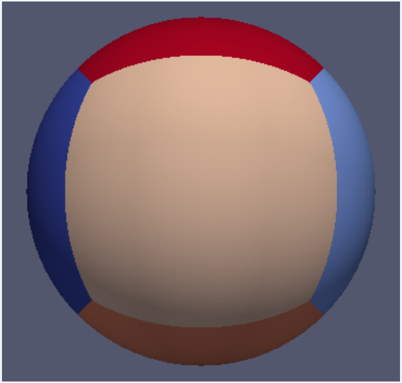
MSc-thesis project by J. Hinz



J. Lefèvre, J-F. Mangin, PLoS Comput. Biol. 6(4) e1000749.

Application: IgA on evolving manifolds

Phenomenological human brain development model



- multi-patch geometry $\Omega_h \simeq \Omega$ approximated by quadratic (hierarchical) B-spline basis functions
- C^{p-1} continuity along patch boundaries due to periodic basis functions
- C^0 continuity in the vicinity of the triple points

Application: IgA on evolving manifolds

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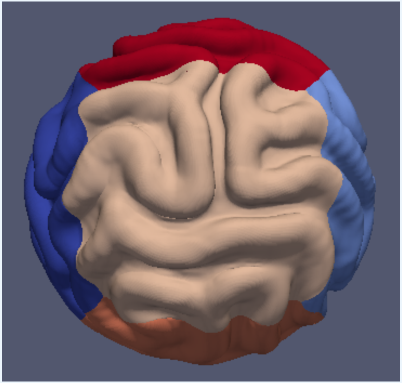

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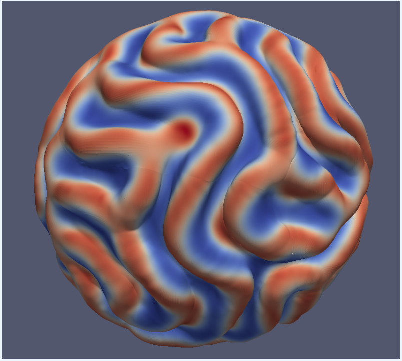
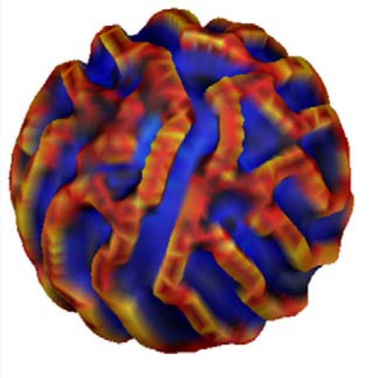
Application: IgA on evolving manifolds

Phenomenological human brain development model





Application: Isogeometric 'mesh generation'[8]

Create a valid mapping (= diffeomorphism, e.g., $\det J > 0$ on Ω_0)

$$\mathbf{G} : \Omega_0 \mapsto \Omega_h \simeq \Omega$$

starting from the boundary parameterization $\bigcup_i \gamma_i$ of Ω by solving

$$\begin{cases} \Delta x(\xi,\eta) & = 0 \\ \Delta y(\xi,\eta) & = 0 \end{cases} \quad \text{s.t.} \quad \mathbf{S}|_{\partial\Omega_i} = \gamma_i.$$

Theory: Ω_h must be convex for $\mathbf{G}$ to be a diffeomorphism.

[8] PhD project by J. Hinz

Application: Isogeometric 'mesh generation'[8]

Create a valid mapping (= diffeomorphism, e.g., $\det J > 0$ on Ω_0)

$$\mathbf{G} : \Omega_0 \mapsto \Omega_h \simeq \Omega$$

starting from the boundary parameterization $\bigcup_i \gamma_i$ of Ω by solving

$$\begin{cases} \Delta\xi(x,y) &= 0 \\ \Delta\eta(x,y) &= 0 \end{cases} \qquad \text{s.t.} \quad \mathbf{S}^{-1}\big|_{\gamma_i} = \partial\Omega_i$$

for the inverse mapping $\mathbf{G}^{-1} : \Omega_h \mapsto \Omega_0$. Inversion yields

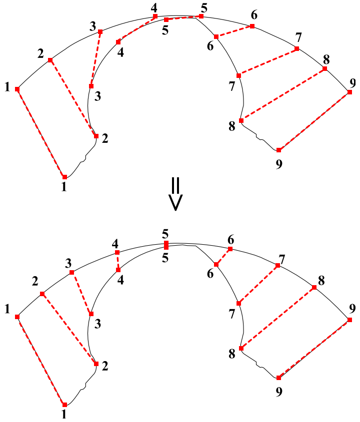
$$\begin{cases} g_{22}x_{\xi\xi} - 2g_{12}x_{\xi\eta} + g_{11}x_{\eta\eta} &= 0 \\ g_{22}y_{\xi\xi} - 2g_{12}y_{\xi\eta} + g_{11}y_{\eta\eta} &= 0 \end{cases} \qquad \text{s.t.} \quad \mathbf{G}\big|_{\partial\Omega_i} = \gamma_i,$$

where $g_{11} = x_\xi^2 + y_\xi^2$, $g_{12} = x_\xi x_\eta + y_\xi y_\eta$ and $g_{22} = x_\eta^2 + y_\eta^2$.

[8] PhD project by J. Hinz

Application: Isogeometric 'mesh generation'[9]

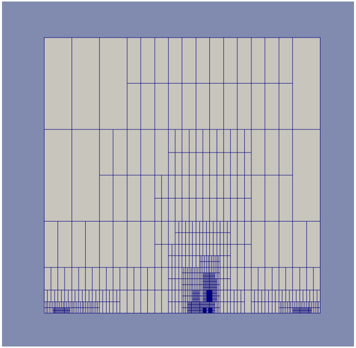
1. Boundary reparameterization



[9] PhD project by J. Hinz

Application: Isogeometric 'mesh generation'[9]

1. Boundary reparameterization
2. Defect detection, e.g., where $\det J(\boldsymbol{\xi}^*) < 0$ or using the dual-weighted residual approach by Becker and Rannacher and refine the parameterization locally (THB-splines by Giannelli *et al.*)



[9] PhD project by J. Hinz

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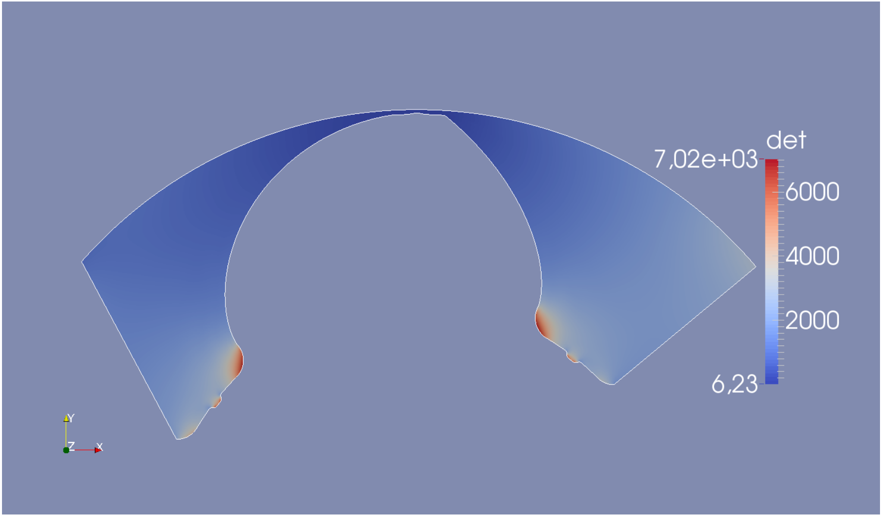
2. Defect detection, e.g., where $\det J(\boldsymbol{\xi}^*) < 0$ or using the dual-weighted residual approach by Becker and Rannacher and refine the parameterization locally (THB-splines by Giannelli *et al.*)

3. Possible extensions:
   - optimization of 'mesh properties'
   - multi-patch segmentation
   - 4th order PDE-problem

[9] PhD project by J. Hinz

Application: Isogeometric 'mesh generation'[9]



[9] PhD project by J. Hinz

Application: Adjoint-based optimization[10]

Proof-of-concept: AD of G+Smo using CoDiPack

$$-\Delta u + \nabla \cdot (\mathbf{v} u) = f \quad \text{in } \Omega_h, \quad u \equiv 1 \quad \text{on } \partial\Omega_h$$

with exact solution $u \equiv 1$.

Goal: Maximize area $A = \|u_h\|_{L^2(\Omega_h)}$ of geometry Ω_h while preserving the circumference $C = \|u_h\|_{L^2(\Gamma_h)}$ of the initial geometry $\Omega_0 = [0,1]^2$.

Gradient based optimization using `IpOpt` with cost functional

$$L = -A + \eta |C_0 - C|$$

[10] PhD project by A. Jaeschke (Lodz)

Conclusion and outlook

1. Open-source Fluid Dynamic Building Blocks library
   `https://gitlab.com/mmoelle1/FDBB.git`
2. IgA-based solver for compressible flows
3. Isogeometric 'mesh generation'
4. Proof-of-concept AD of G+Smo code

Ongoing and future work:

- Distributed JIT compilation of multi-patch geometries
- Embedding of linear algebra SFETs into CoDiPack
- Extension towards FPGAs (reconfigurable computing)

Appendix

Further applications of the AFC framework

Idealized Z-pinch implosion model[11]

- Generalized Euler system coupled with scalar tracer equation

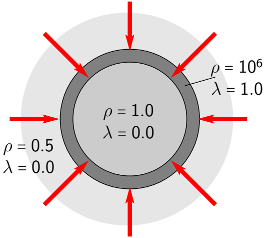
$$\frac{\partial}{\partial t}\begin{bmatrix}\rho \\ \rho\mathbf{v} \\ \rho E \\ \rho\lambda\end{bmatrix} + \nabla\cdot\begin{bmatrix}\rho\mathbf{v} \\ \rho\mathbf{v}\otimes\mathbf{v} + p\mathcal{I} \\ \rho E\mathbf{v} + p\mathbf{v} \\ \rho\lambda\mathbf{v}\end{bmatrix} = \begin{bmatrix}0 \\ \mathbf{f} \\ \mathbf{f}\cdot\mathbf{v} \\ 0\end{bmatrix}$$

- Equation of state

$$p = (\gamma - 1)\rho(E - 0.5|\mathbf{v}|^2)$$

- Non-dimensional Lorentz force

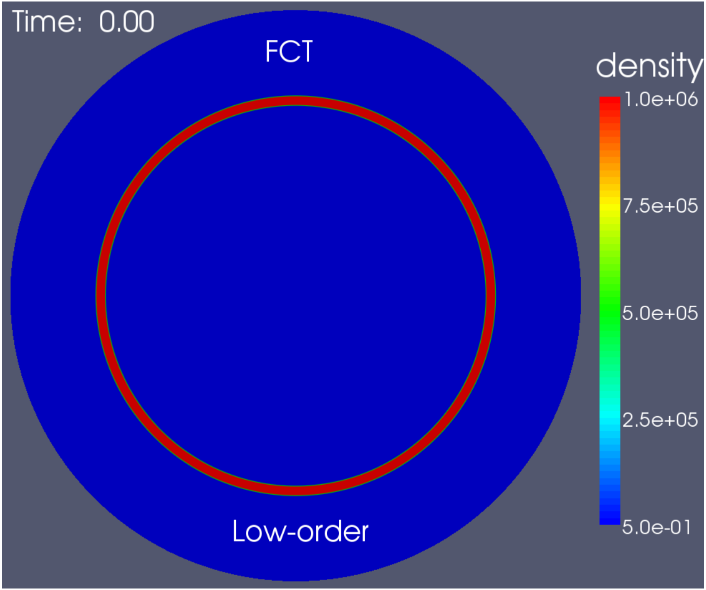
$$\mathbf{f} = (\rho\lambda)\left(\frac{I(t)}{I_{\max}}\right)^2 \frac{\hat{\mathbf{e}}_r}{r_{\text{eff}}}, \quad 0 \le \lambda \le 1$$



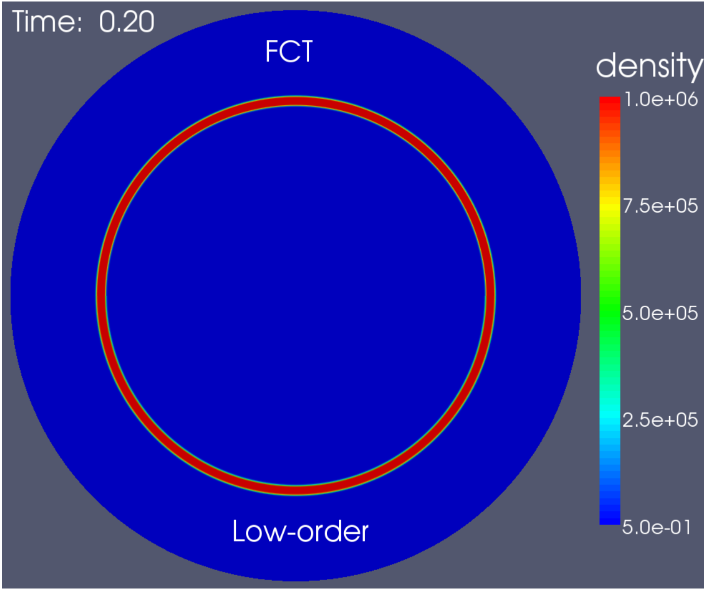
$\mathbf{v} = 0.0$, $p = 1.0$ everywhere

[11] J.W. Banks, J.N. Shadid, IJNMF 2009, 61(7), 725–751

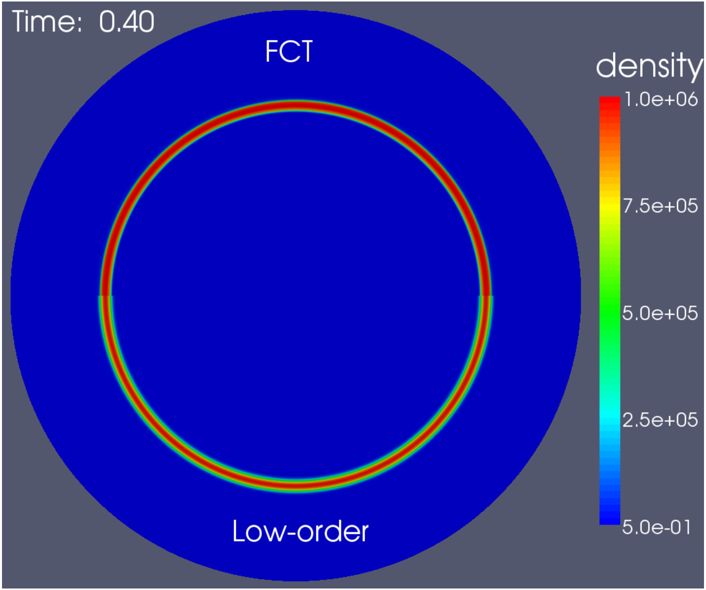
Idealized Z-pinch implosion



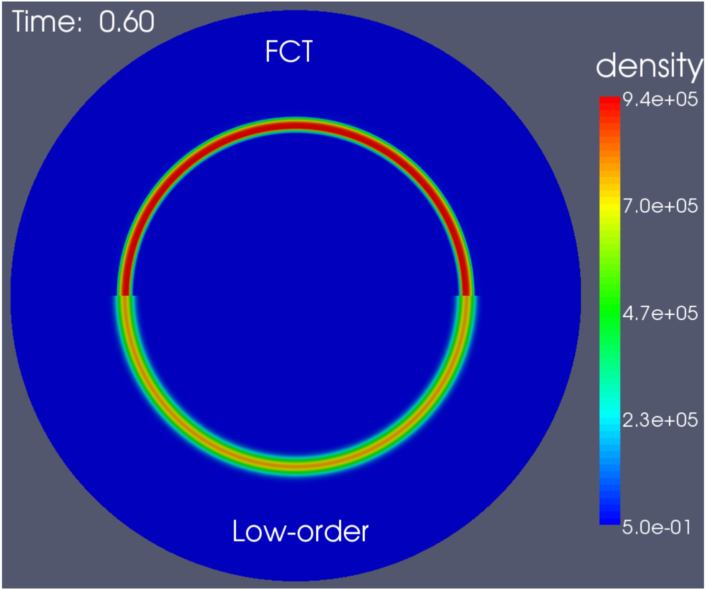
Idealized Z-pinch implosion



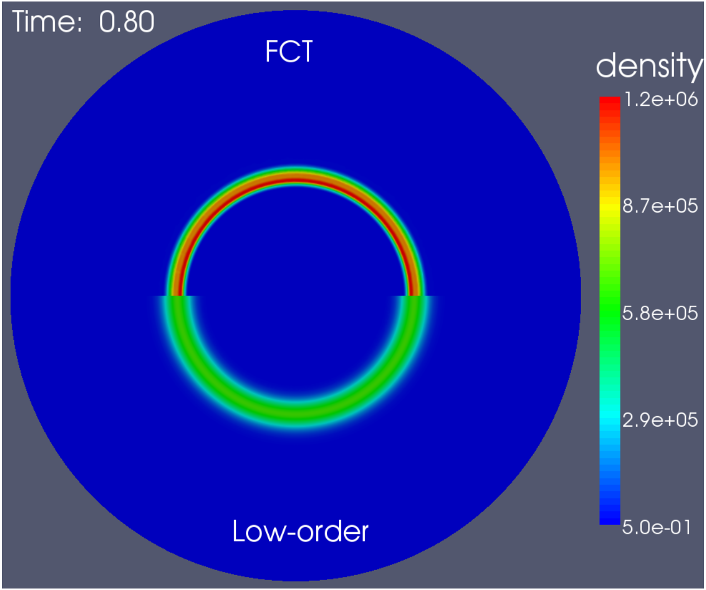
Idealized Z-pinch implosion



Idealized Z-pinch implosion



Idealized Z-pinch implosion



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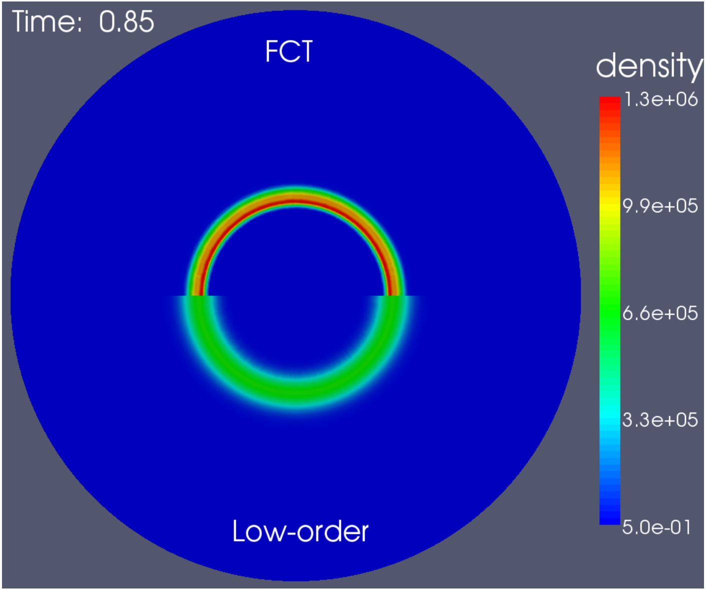

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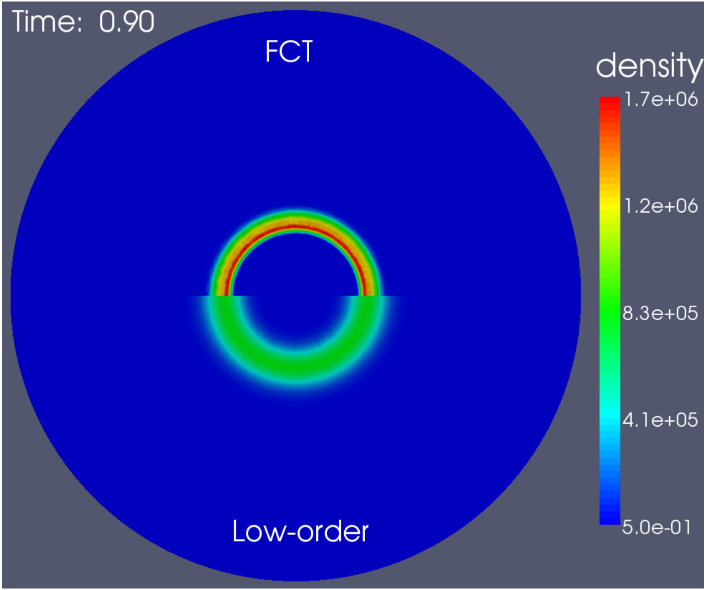
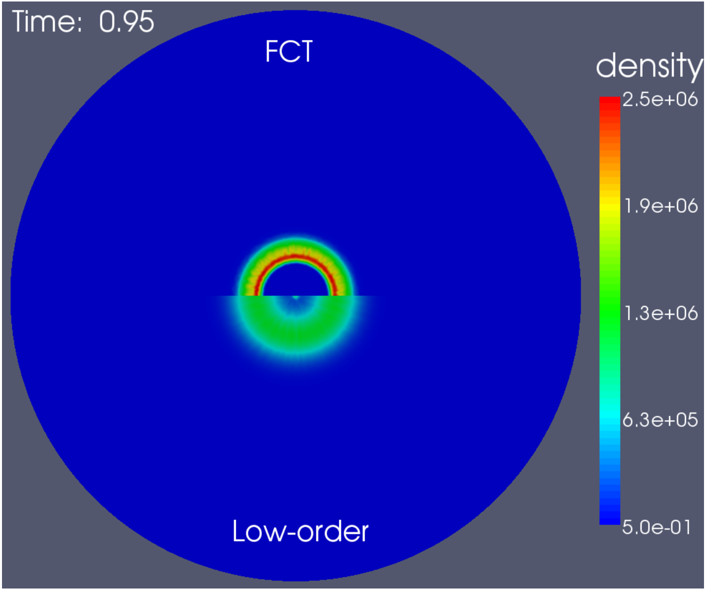


Idealized Z-pinch implosion



Idealized Z-pinch implosion