Steady-state Flow Simulations using Exact Jacobians on Cartesian Grids

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Outline

- Introduction
- Different Approaches for Jacobians
  - Finite Differences
  - Automatic Differentiation
  - Analytic Differentiation
- Numerical Results
- Outlook

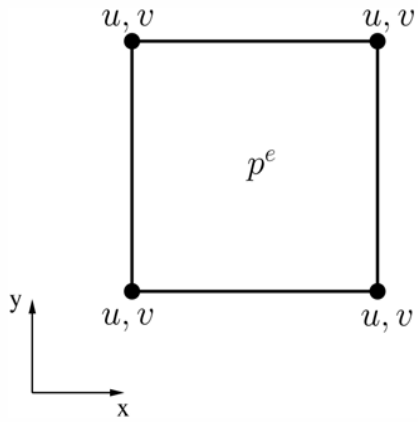
Introduction

- Incompressible Navier-Stokes equations (NSE)

$$\begin{aligned} \dot{\mathbf{u}} + (\mathbf{u} \cdot \nabla)\mathbf{u} + \frac{1}{\mathrm{Re}}\Delta\mathbf{u} - \nabla p &= \mathbf{0} \\ \nabla \cdot \mathbf{u} &= 0 \end{aligned}$$

- Discretisation in Peano framework
  - Low-order FEM (Q1P0)
  - Steady-state: preparation for implicit time integration
  - Discrete NSE:

$$\begin{aligned} C(\mathbf{u}_h)\mathbf{u}_h + D\mathbf{u}_h - M^T p_h &= \mathbf{0} \\ M\mathbf{u}_h &= 0 \end{aligned}$$



Introduction

- Nonlinear system of equations

$$\begin{aligned} C(\mathbf{u}_h)\mathbf{u}_h + D\mathbf{u}_h - M^T p_h &= \mathbf{0} \\ M\mathbf{u}_h &= 0 \end{aligned} \quad \Leftrightarrow \quad 0 = B(\mathbf{u}_h, p_h) =: B(u) \in \mathbf{R}^N$$

- Newton's method (PETSc)

$$\begin{aligned} k &= 0, 1, \ldots \\ J(u_k) \cdot \Delta u_k &= -B(u_k) \\ u_{k+1} &= u_k + \Delta u_k \end{aligned}$$

- Initial value
  - Crucial for convergence
  - Pseudo-timestepping (semi-implicit, PPE)

Introduction

- Nonlinear system of equations

$$\begin{aligned} C(\mathbf{u}_h)\mathbf{u}_h + D\mathbf{u}_h - M^T p_h &= \mathbf{0} \\ M\mathbf{u}_h &= 0 \end{aligned} \quad \Leftrightarrow \quad 0 = B(\mathbf{u}_h, p_h) =: B(u) \in \mathbf{R}^N$$

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- Initial value
  - Crucial for convergence
  - Pseudo-timestepping (semi-implicit, PPE)

Jacobian - Finite Differences

- FD untuned
  - Use default B evaluation
  - Very (!) slow

$$J(u,\varepsilon)_i \approx \frac{B(u+\varepsilon\cdot e_i)-B(u)}{\varepsilon}$$

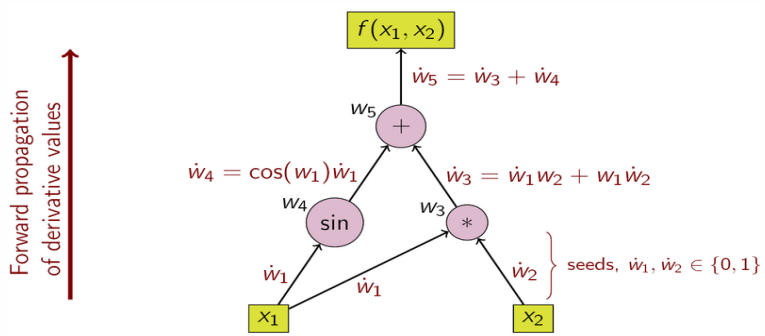
$$\varepsilon = \begin{cases} 10^{-8}\cdot u_i & \text{if } |u_i| > 10^{-8} \\ 10^{-8}\cdot 10^{-8}\cdot sign(u_i) & \text{otherwise} \end{cases}$$

- FD (tuned)
  - Manual implementation (no default B evaluation)
  - Avoid unnecessary operator evaluations (due to stencil)

Jacobian - Automatic Differentiation

- Apply chaine rule for derivatives computationally
  - Example: Forward accumulation $f(x_1, x_2) = x_1 \cdot x_2 + \sin(x_1)$

Original code statements	Added statements for derivatives
$w_1 = x_1$	$w'_1 = 1$ (seed)
$w_2 = x_2$	$w'_2 = 0$ (seed)
$w_3 = w_1 w_2$	$w'_3 = w'_1 w_2 + w_1 w'_2 = 1 x_2 + x_1 0 = x_2$
$w_4 = \sin(w_1)$	$w'_4 = \cos(w_1) w'_1 = \cos(x_1) 1$
$w_5 = w_3 + w_4$	$w'_5 = w'_3 + w'_4 = x_2 + \cos(x_1)$



Source: www.wikipedia.org

  - Backward accumulation
  - Mixed
- Realisation in AD tools
  - Source code transformation (function.cpp ➔ diff_function.cpp)
  - Operator overloading (special data type)

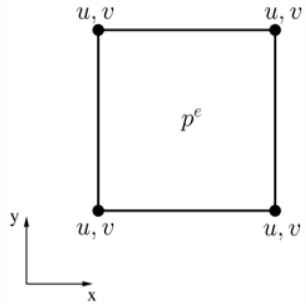
Jacobian - Automatic Differentiation

Package	Mode	Version	Positive	Negative	misc
ADC	Operator overloading (forward)	unknown	probably efficient	not used widely	commercial
ADIC	Source transformation (forward)	Jun 2005	-	Win32 not supported community dead bad documenation	registration necessary
ADOL-C	**Operator overloading (forward,backward)**	**Aug 2006**	**all OS supported good documentation many features (Jacobian, sparsity) active community**	**-**	**by TU Dresden**
COSY INFINITY	Operator overloading (forward)	2006	all OS supported good documenation suitable for high-dim sparsity features	no community free for private use	registration necessary
CppAD	Operator overloading (forward, backward)	Mar 2008	all OS supproted good documentation integrated speed tests sparsity features	-	-
FAD	Operator overloading (forward)	2002	-	Win32 not supported community dead bad documentation	-
FADBAD++	Operator overloading (forward, backward)	unknown	all OS supported documentation ok	no community little information	-
FFADLib	Operator overloading (forward)	unknown	-	Unix not supported	registration necessary
OpenAD	Source Transformation (forward, backward)	Nov 2006	good documentation	Win32 not supported uses external libs	used by NASA
YAO	unknown (forward, backward)	unknwon	-	Win32 not supported no information	website in French

www.autodiff.org

Jacobian – Analytic Differentiation

$$B\begin{pmatrix}\mathbf{u}_h\\ p_h\end{pmatrix} := \begin{pmatrix}\underbrace{C(\mathbf{u}_h)\,\mathbf{u}_h + D\mathbf{u}_h}_{=:F} + M^T p_h\\ M\mathbf{u}_h\end{pmatrix} = \mathbf{0}$$

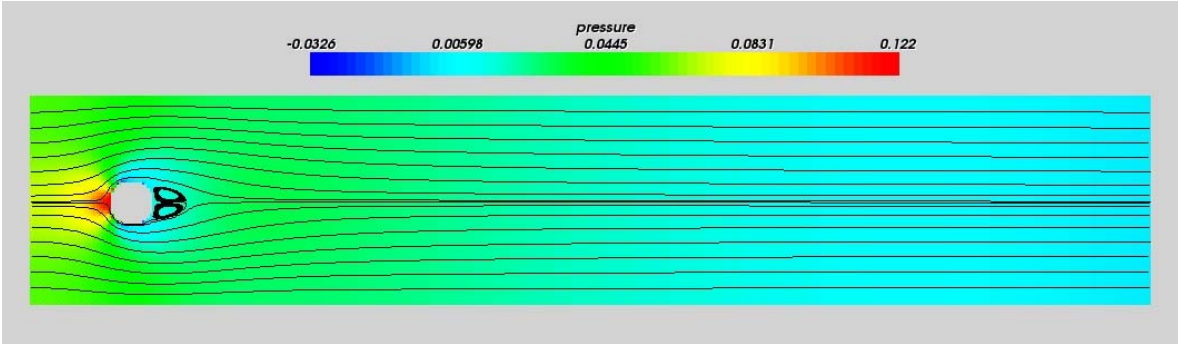


- Block 1: linear
- Block 2: linear
- Block 3: non-linear

$$J^e = \left(\begin{array}{c|c} \text{Block 3}\ \frac{\partial F}{\partial \mathbf{u}_h} & \text{Block 2}\ \frac{\partial \nabla_h}{\partial p_h} \\ \hline \text{Block 1}\ \frac{\partial \nabla_h}{\partial \mathbf{u}_h} & 0 \end{array}\right) \in \mathbf{R}^{9\times 9}$$

Numerical Results

- Benchmark scenario: Laminar flow around a cylinder 1)
  - Lift and drag forces for comparison
  - Regular Cartesian grids
  - Re = 20



- PETSc solver
  - Explicit assemblation of J
  - GMRES + ILU
  - rtol = atol = 1e-7

1) S. Turek and M. Schaefer, “Benchmark Computations of Laminar Flow around a Cylinder” Vieweg, Notes on Numerical Fluid Mechanics 52, 1996

Numerical Results - I

compiled w/o ADOL-C	time total	time J	time B	lin. it. total	lin. iterations per non-lin. it.	c_d 4.9561	c_l 0.0210
FD							
1 step	53.0	0.8	0.04	1335	209 - 556 - 322 - 191 - 57	4.9561	0.0210
2 steps	21.8	0.8	0.04	231	105 - 65 - 43 - 18	4.9561	0.0210
10 steps	24.0	0.8	0.04	202	92 - 56 - 43 - 11	4.9561	0.0210
ANALYTICAL							
1 step	48.9	0.12	0.04	1309	182 - 556 - 323 - 191 - 57	4.9561	0.0210
2 steps	19.4	0.12	0.04	231	105 - 65 - 43 - 18	4.9561	0.0210
10 steps	21.5	0.12	0.04	202	92 - 56 - 43 - 11	4.9561	0.0210

220x41

N=26,406

Numerical Results - I

Untuned FD:

Time J = 1198

compiled w/o ADOL-C	time total	time J	time B	lin. it. total	lin. iterations per non-lin. it.	c_d 4.9561	c_l 0.0210
FD							
1 step	53.0	0.8	0.04	1335	209 - 556 - 322 - 191 - 57	4.9561	0.0210
2 steps	21.8	0.8	0.04	231	105 - 65 - 43 - 18	4.9561	0.0210
10 steps	24.0	0.8	0.04	202	92 - 56 - 43 - 11	4.9561	0.0210
ANALYTICAL							
1 step	48.9	0.12	0.04	1309	182 - 556 - 323 - 191 - 57	4.9561	0.0210
2 steps	19.4	0.12	0.04	231	105 - 65 - 43 - 18	4.9561	0.0210
10 steps	21.5	0.12	0.04	202	92 - 56 - 43 - 11	4.9561	0.0210

220x41

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Numerical Results - I

compiled w/o ADOL-C	time total	time J	time B	lin. it. total	lin. iterations per non-lin. it.	c_d 4.9561	c_l 0.0210
FD							
1 step	53.0	0.8	0.04	1335	209 - 556 - 322 - 191 - 57	4.9561	0.0210
2 steps	21.8	0.8	0.04	231	105 - 65 - 43 - 18	4.9561	0.0210
10 steps	24.0	0.8	0.04	202	92 - 56 - 43 - 11	4.9561	0.0210
ANALYTICAL							
1 step	48.9	0.12	0.04	1309	182 - 556 - 323 - 191 - 57	4.9561	0.0210
2 steps	19.4	0.12	0.04	231	105 - 65 - 43 - 18	4.9561	0.0210
10 steps	21.5	0.12	0.04	202	92 - 56 - 43 - 11	4.9561	0.0210

220x41

N=26,406

compiled with ADOL-C	time total	time J	time B	lin. it. total	lin. iterations per non-lin. it.	c_d 4.9561	c_l 0.02108
FD							
1 step	83.0	6.45	0.21	1337	211 - 556 - 322 - 191 - 57	4.9561	0.02108
2 steps	45.6	6.45	0.21	231	105 - 65 - 43 - 18	4.9561	0.02108
10 steps	49.8	6.45	0.21	202	92 - 56 - 43 - 11	4.9561	0.02108
ANALYTICAL							
1 step	50.3	0.12	0.21	1309	182 - 556 - 323 - 191 - 57	4.9561	0.02108
2 steps	20.5	0.12	0.21	231	105 - 65 - 43 - 18	4.9561	0.02108
10 steps	24.0	0.12	0.21	202	92 - 56 - 43 - 11	4.9561	0.02108
ADOL-C							
1 step	54.7	0.98	0.21	1309	182 - 556 - 323 - 191 - 57	4.9561	0.02108
2 steps	24.1	0.98	0.21	231	105 - 65 - 43 - 18	4.9561	0.02108
10 steps	27.6	0.98	0.21	202	92 - 56 - 43 - 11	4.9561	0.02108

ADOL-C datatype

(operator overloading)

Numerical Results - I

compiled w/o ADOL-C	time total	time J	time B	lin. it. total	lin. iterations per non-lin. it.	c_d 4.9561	c_l 0.0210
FD							
1 step	53.0	0.8	0.04	1335	209 - 556 - 322 - 191 - 57	4.9561	0.0210
2 steps	21.8	0.8	0.04	231	105 - 65 - 43 - 18	4.9561	0.0210
10 steps	24.0	0.8	0.04	202	92 - 56 - 43 - 11	4.9561	0.0210
ANALYTICAL							
1 step	48.9	0.12	0.04	1309	182 - 556 - 323 - 191 - 57	4.9561	0.0210
2 steps	19.4	0.12	0.04	231	105 - 65 - 43 - 18	4.9561	0.0210
10 steps	21.5	0.12	0.04	202	92 - 56 - 43 - 11	4.9561	0.0210

compiled with ADOL-C	time total	time J	time B	lin. it. total	lin. iterations per non-lin. it.	c_d 4.9561	c_l 0.02108
FD							
1 step	83.0	6.45	0.21	1337	211 - 556 - 322 - 191 - 57	4.9561	0.02108
2 steps	45.6	6.45	0.21	231	105 - 65 - 43 - 18	4.9561	0.02108
10 steps	49.8	6.45	0.21	202	92 - 56 - 43 - 11	4.9561	0.02108
ANALYTICAL							
1 step	50.3	0.12	0.21	1309	182 - 556 - 323 - 191 - 57	4.9561	0.02108
2 steps	20.5	0.12	0.21	231	105 - 65 - 43 - 18	4.9561	0.02108
10 steps	24.0	0.12	0.21	202	92 - 56 - 43 - 11	4.9561	0.02108
ADOL-C							
1 step	54.7	0.98	0.21	1309	182 - 556 - 323 - 191 - 57	4.9561	0.02108
2 steps	24.1	0.98	0.21	231	105 - 65 - 43 - 18	4.9561	0.02108
10 steps	27.6	0.98	0.21	202	92 - 56 - 43 - 11	4.9561	0.02108

220x41

N=26,406

Numerical Results - II

compiled w/o ADOL-C	time total	time J	time B	lin. it. total	lin. iterations per non-lin. it.	c_d 4.7094	c_l 0.01107
FD							
2 steps	177.3	3.44	0.14	606	324 - 146 - 112 - 24	4.7094	0.01108
10 steps	173.4	3.44	0.14	500	223 - 147 - 102 - 28	4.7094	0.01108
100 steps	201.9	3.44	0.14	425	178 - 138 - 103 - 6	4.7094	0.01107
ANALYTICAL							
2 steps	162.9	0.49	0.14	590	306 - 147 - 103 - 24	4.7094	0.01108
10 steps	160.9	0.49	0.14	500	223 - 147 - 102 - 28	4.7094	0.01108
100 steps	194.1	0.49	0.14	474	226 - 139 - 104 - 5	4.7094	0.01107

compiled with ADOL-C	time total	time J	time B	lin. it total	lin. iterations per non-lin. it.	c_d 4.7094	c_l 0.01107
FD							
2 steps	266.8	25.95	0.84	577	293 - 147 - 113 - 24	4.7094	0.01108
10 steps	274.0	25.95	0.84	500	223 - 147 - 102 - 28	4.7094	0.01108
100 steps	362.9	25.95	0.84	425	178 - 138 - 103 - 6	4.7094	0.01107
ANALYTICAL							
2 steps	165.6	0.49	0.84	590	306 - 147 - 103 - 24	4.7094	0.01108
10 steps	170.7	0.49	0.84	500	223 - 147 - 102 - 28	4.7094	0.01108
100 steps	268.4	0.49	0.84	474	226 - 139 - 104 - 5	4.7094	0.01107
ADOL-C							
2 steps	178.6	3.72	0.84	590	306 - 147 - 103 - 24	4.7094	0.01108
10 steps	184.8	3.72	0.84	500	223 - 147 - 102 - 28	4.7094	0.01108
100 steps	280.2	3.72	0.84	474	226 - 139 - 104 - 5	4.7094	0.01107

440x82

N=106,622

ADOL-C datatype

(operator overloading)

Numerical Results - III

compiled with ADOL-C	time total	time J	time B	lin. it total	lin. iterations per non-lin. it.	c_d 4.6112	c_l 0.00525
FD 2 steps	1310.1	7.45	0.31	3733	2876 - 475 - 328 - 54	4.6112	0.00525
ANALYTICAL 2 steps	1292.3	1.17	0.31	3849	2959 - 473 - 327 - 90	4.6112	0.00526
ADOL-C 2 steps	1318.7	8.74	1.95	3812	2956 - 474 - 328 - 54	4.6112	0.00526

660x123

N=240,670

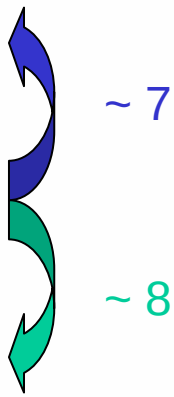
Numerical Results - III

compiled with ADOL-C	time total	time J	time B	lin. it total	lin. iterations per non-lin. it.	c_d 4.6112	c_l 0.00525
FD 2 steps	1310.1	7.45	0.31	3733	2876 - 475 - 328 - 54	4.6112	0.00525
ANALYTICAL 2 steps	1292.3	1.17	0.31	3849	2959 - 473 - 327 - 90	4.6112	0.00526
ADOL-C 2 steps	1318.7	8.74	1.95	3812	2956 - 474 - 328 - 54	4.6112	0.00526

660x123

N=240,670

time J	220	4	440	2.25	660
FD	**0.8**	4.2	**3.4**	2.2	**7.45**
	6.6		7		6.4
ANALYTICAL	**0.12**	4	**0.49**	2.4	**1.17**
	8		7.5		7.5
ADOL-C	**0.98**	3.8	**3.72**	2.3	**8.74**

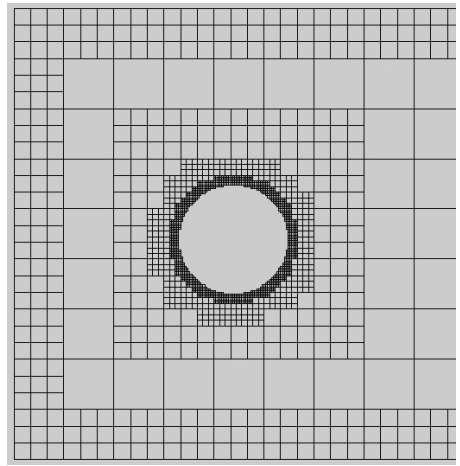


Conclusion

Criterion	FD	ADOLC	ANALYTICAL
Easy to implement	0	0	0
No code duplication	-	+	-
No manual choice of ε	-	+	+
Less non-lin. its	0	+?	+?
Less linear its	0	+?	+?
Runtime Jacobian	-	-	+
Runtime B (+ pseudo-timestepping)	+	- -	+

Outlook

- ADOL-C tapeless
  - Faster
  - N fixed at compile time
- Matrix-free
  - All 3 approaches for Jacobian usable
  - Element-wise matrix-vector multiplication
  - No preconditioning ➔ use built-in geometric multigrid when available
- 3D
  - Implementation completed (all 3 approaches)
  - Convergence problems (ILU)
- Implicit time integration
  - Euler
  - Trapezoidal rule
- Adaptive grids

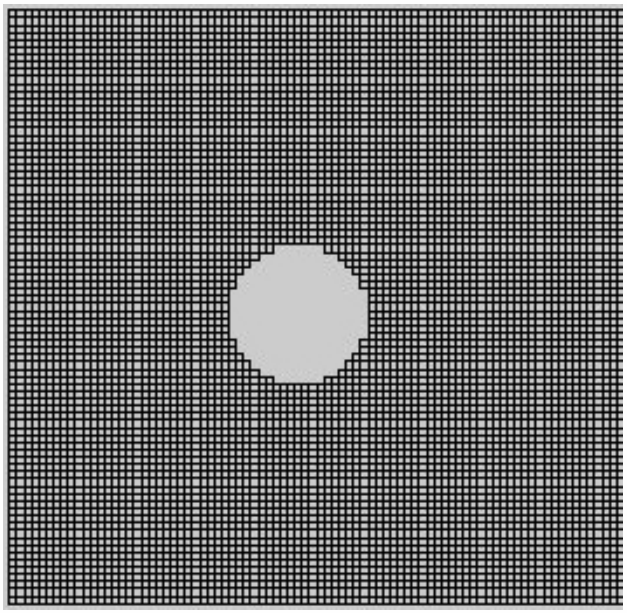


Thanks for your attention!

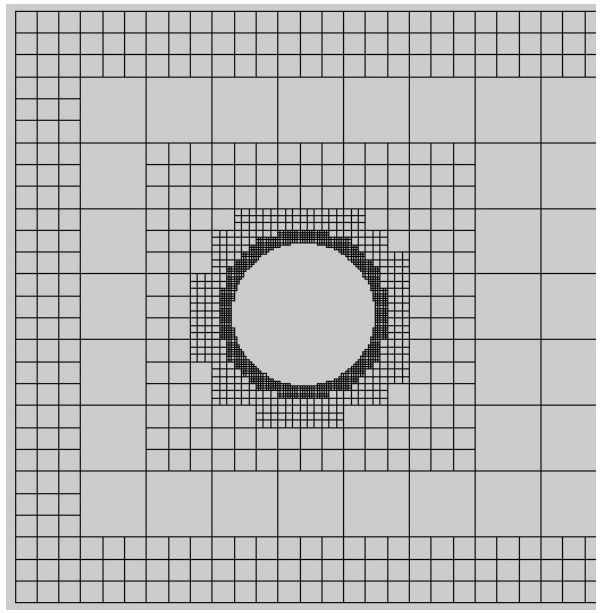
Backup - Peano

- Framework for different applications (Poisson, NSE, etc.): “plug-in concept”
- Cartesian grids + cell-wise operator evaluation

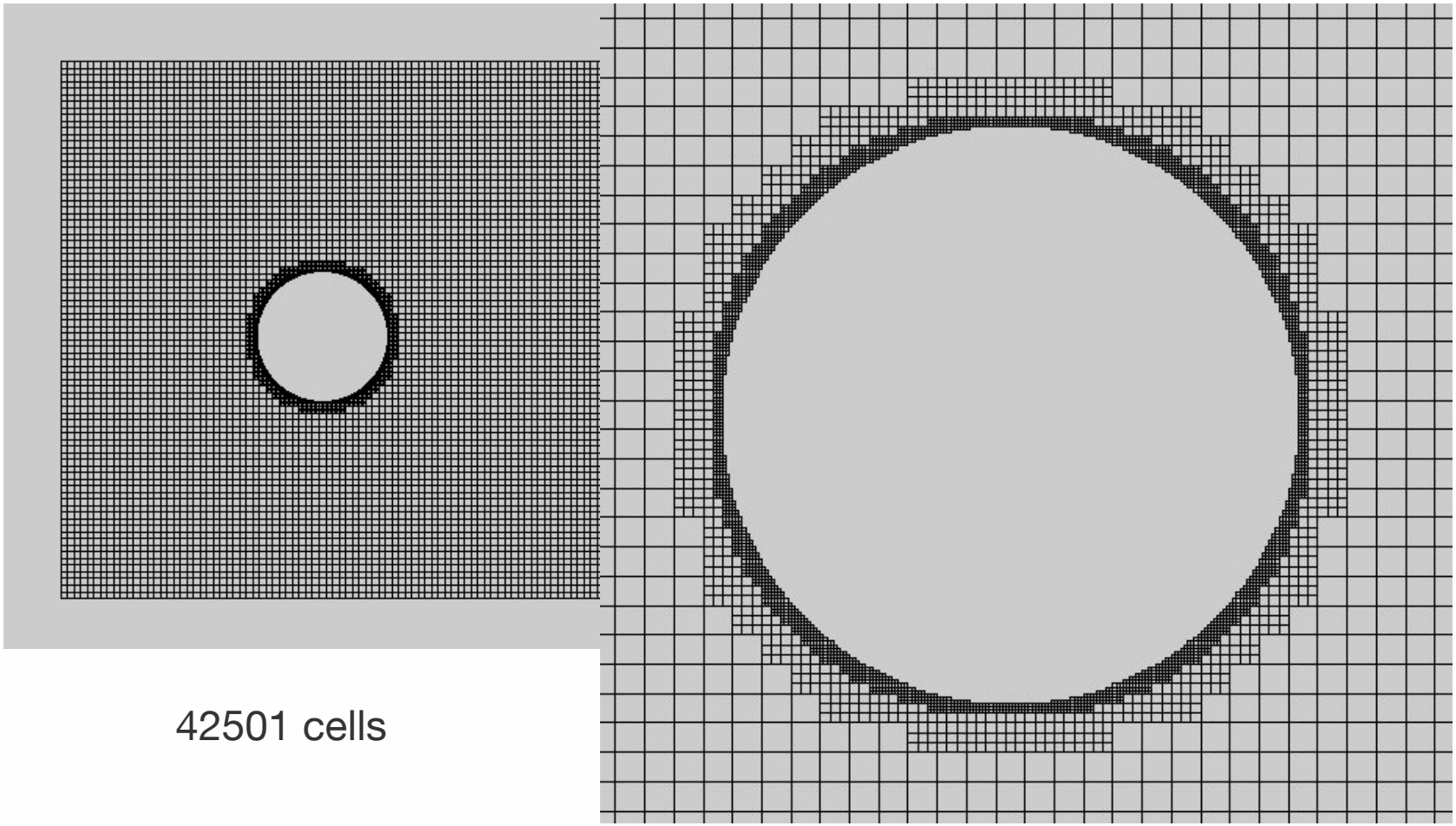
Regular (lexicographic)



Adaptive (spacetree)

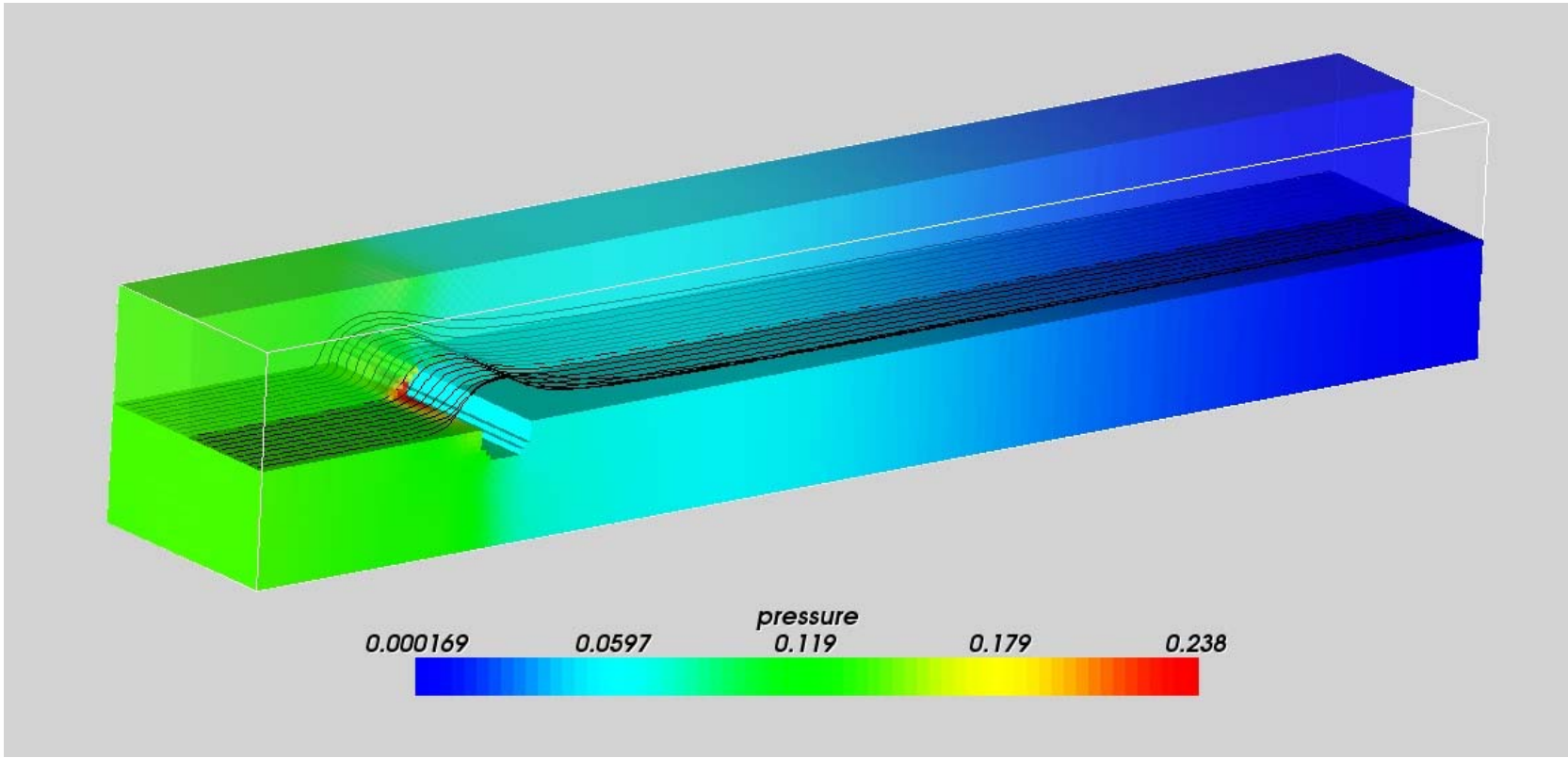


Backup – Adaptive Grid



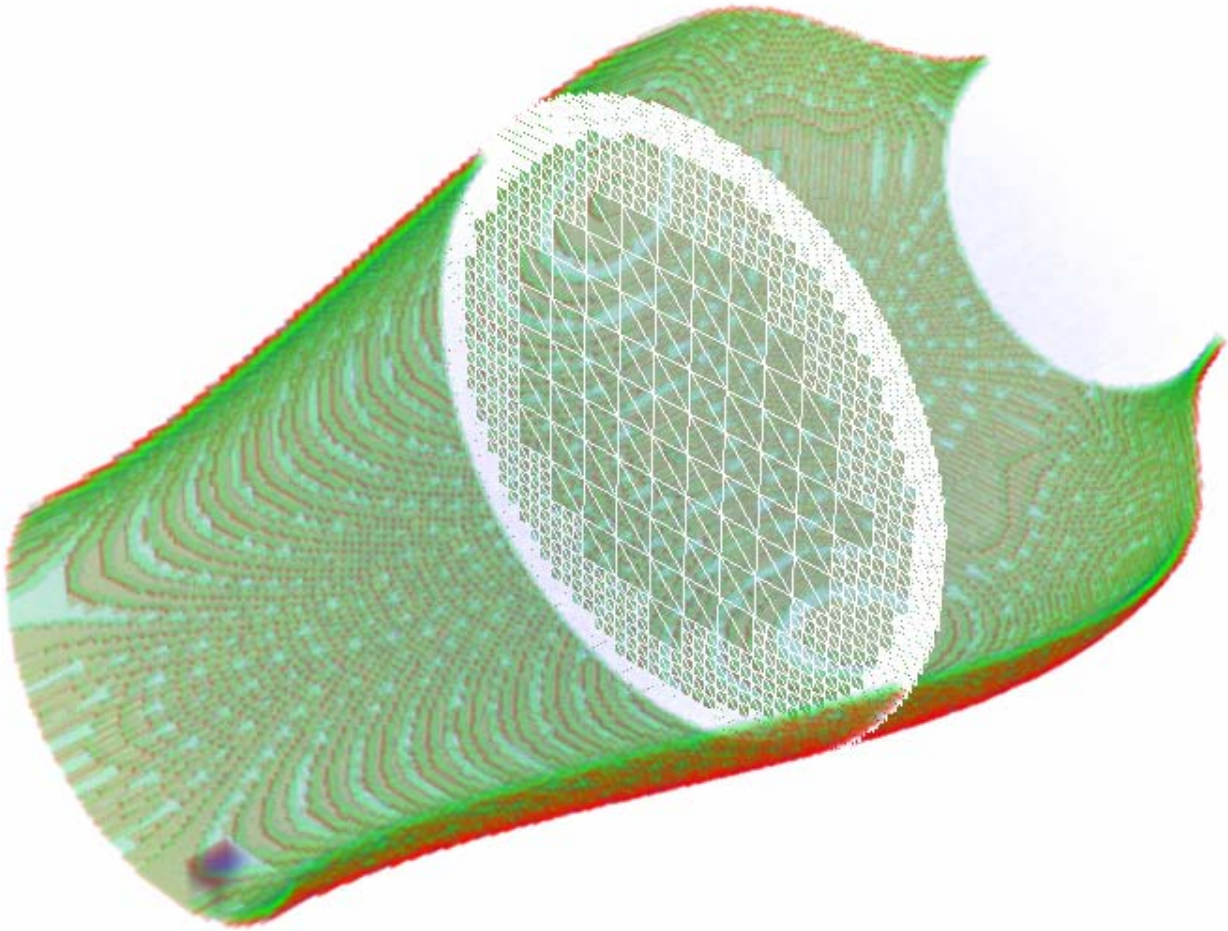
42501 cells

Backup II – Cylinder Benchmark 3D



416642 cells

Backup III – 3D adaptive Drift-Ratchet



Backup IV – Peano Architecture