Efficient on-the-fly Operator Assembly for HPC Finite Element Codes

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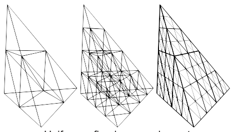
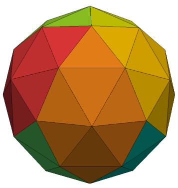
Software Framework - Hierarchical Hybrid Grids (HHG) [1]

- Unstructured macro mesh
- Uniform refinement of macro elements
- Primitive based data structures + ghost layer exchange
- Matrix-free implementation (on-the-fly stencil assembly)

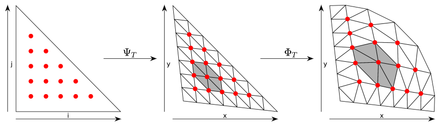


Uniform refined macro element

Problem: On-the-fly stencil assembly on curved domains requires expensive evaluation of local element matrices over and over again.

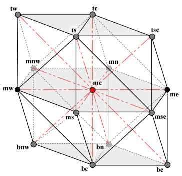


Initial macro triangulation of spherical shell geometry



2D sketch of sequence of mappings for curved domains

Novel Approach - FE Stencil Approximation

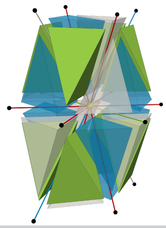


LSQP (least-squares polynomial) [2]

Replace each component of 15pt stencil by a quadratic polynomial. Compute polynomial coefficients in setup phase by least-squares fit. Do this for each macro element.

+ very fast
+ accuracy is $O(h^2) + O(H^3)$ (for linear FE with element length h and macro element length H)
- for PDEs with a variable material parameter this is only applicable, if the parameter is sufficiently smooth

Extension for PDEs with variable material parameter



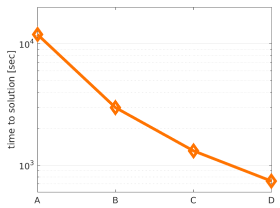
LSQP LocEl (local elements)

Replace entries of local element matrices by polynomial approximations. Use these approximations and the material parameter to assemble the stencils in a standard way.

- requires more FLOPs than LSQP, but still much faster than computing local element matrices via quadrature rules
+ technique is applicable to PDEs with general material parameters
+ for constant material parameter it is equivalent to LSQP

LSQP LocEL for Stokes-type PDE with variable viscosity - Performance Results on SuperMUC Phase1

Optimization Steps

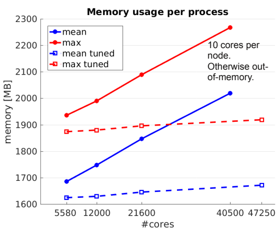


Time to solution for system with $O(10^{10})$ DOFs using 1920 cores

A) standard on-the-fly FE stencil assembly
B) LSQP LocEl
C) B + store stencils on lower dimensional primitives (faces)
D) C + optimized polynomial evaluation

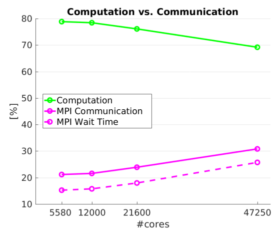
LSQP LocEl 16x faster than standard FE assembly

Weak Scaling on up to 47 250 cores with $2.3\cdot 10^7$ DOFs per core

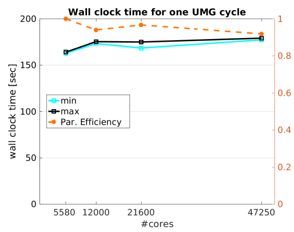


Optimized memory usage with tuned MPI buffer sizes

I_MPI_DAPL_UD_SEND_BUFFER_NUM=8208
I_MPI_DAPL_UD_RECV_BUFFER_NUM=8208
I_MPI_DAPL_UD_ACK_SEND_POOL_SIZE=8704
I_MPI_DAPL_UD_ACK_RECV_POOL_SIZE=8704
I_MPI_DAPL_UD_RNDV_EP_NUM=2



Excludes all initialization times. Only moderate increase of MPI communication. Most of the execution time is spent in compute-intense smoothing kernel.



Excellent parallel efficiency of more than 90% on up to 47 250 compute cores

Geophysical Application at Extreme Scale - Global Resolution of ~ 1.7 km

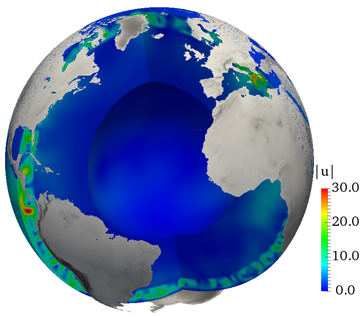
Governing equations

$$-\operatorname{div}(2\mu\dot{\varepsilon}(\mathbf{u})) + \nabla p = -\rho\mathbf{g}$$
$$\operatorname{div}\mathbf{u} = 0$$

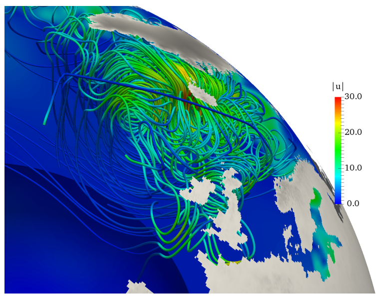
- Temperature dependent viscosity profile with jump at 660km depth (assumed to be bottom end of the asthenosphere)

$$\mu(\mathbf{x},T)=\exp\left(4.61\frac{1-\|\mathbf{x}\|_2}{1-r_{\text{cmb}}}-2.99T\right)\begin{cases}1/10\cdot 6.371^3 d_a^3 & \text{for } \|\mathbf{x}\|_2>1-d_a,\\ 1 & \text{else.}\end{cases}$$

- Present day temperature and density field [3,4]
- Platevelocities [5] at surface and freeslip boundary conditions at core mantle boundary (cmb)
- Global 1.7km resolution yields system with $O(10^{12})$ DOFs



Avg. velocity whole mantle	2.92 [cm/a]
Avg. velocity asthenosphere	7.02 [cm/a]
Avg. velocity lower mantle	2.10 [cm/a]
Max velocity asthenosphere	42.46 [cm/a]
Max velocity lower mantle	12.40 [cm/a]



Velocity streamlines at Iceland plume

Accuracy: Standard on-the-fly FE stencil assembly vs. LSQP LocEl
Average velocities differ by less than 3% and maximal velocities by even less than 1%.

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