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h-type adaptive mesh refinement for spectral element solvers. Application to Nek5000 and Neko

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Outline

- Introduction
- Spectral element method
- Adaptive mesh refinement
- Nek5000 implementation
- Current work on Neko

Introduction

- Presented material is a result of work supported by multiple EU projects : CRESTA, ExaFLOW and EXCELLERAT
- There are two current EU project focusing on Neko and adaptive mesh refinement: CEEC and EXCELLERAT P2
  - Relatively big project, so collaboration needed

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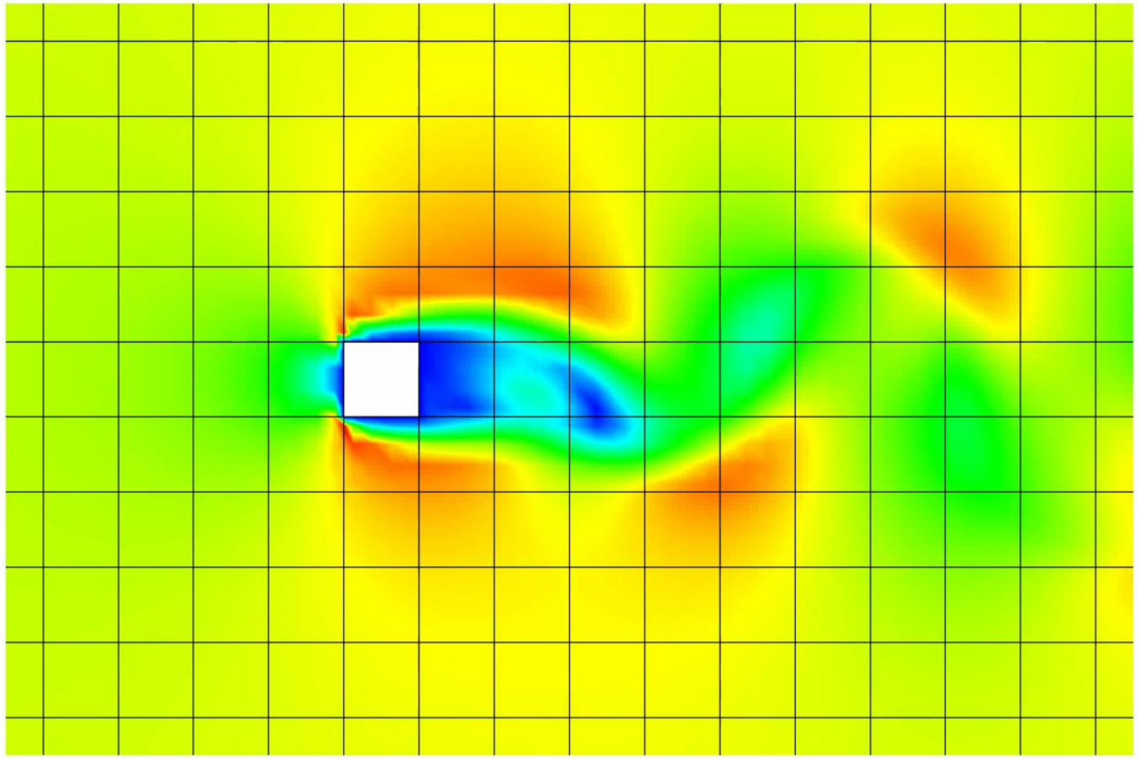
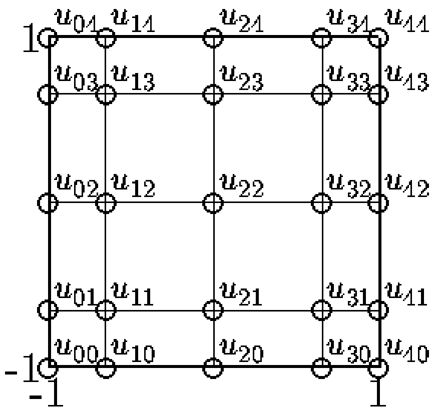
Introduction



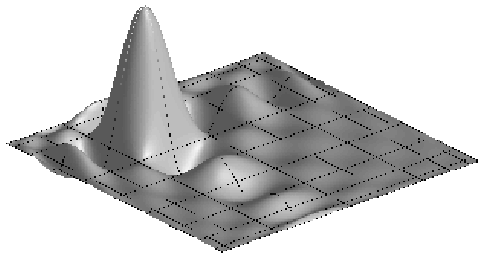
- Exascale simulations:
  - Pose problem for meshing
  - Unknown physics
  - Reliability of simulation data
- Specific goals
  - Resolve sensitive regions
  - Quality assessment/assurance of data
  - Reduced computational cost
- Required tools
  - Grid management library
  - Load balancing/grid repartitioning
  - Refinement indicator/error estimators
  - Solver for non-conformal meshes

Spectral element method

- Variational method, similar to FEM, using GL quadrature
- Domain partitioned into $\boldsymbol{E}$ high-order **hexahedral elements**
- Trial and test functions represented as $\boldsymbol{N}$th-order **tensor-product polynomials** within each element.
- Converges **exponentially fast** with $\boldsymbol{N}$ for smooth solutions.



N=4



N=10

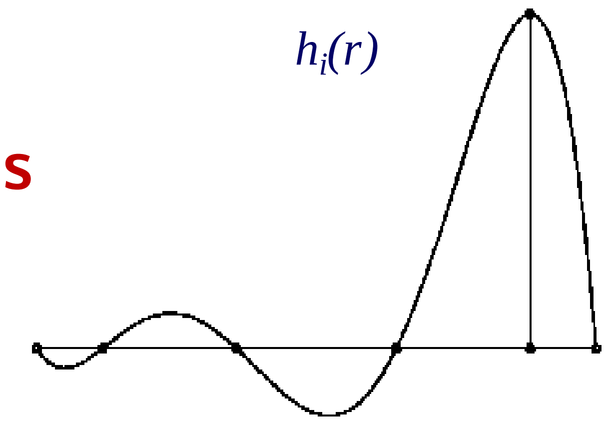
Deville et al 2002

$$u(x,y) = \sum_{i=0}^{N} \sum_{j=0}^{N} u_{ij} h_i(x) h_j(y), \;\; h_i(\xi_p) = \delta_{ip}, \;\; h_i \in \mathbb{P}_N$$

Spectral element method

Local tensor-product form (2D),

$$u(r,s)=\sum_{i=0}^{N}\sum_{j=0}^{N}u_{ij}h_i(r)h_j(s), \quad h_i(\xi_p)=\delta_{ip},\ h_i\in\mathbb{P}_N$$



Deville et al 2002

allows derivatives to be evaluated as **matrix-matrix products**

$$\left.\frac{\partial u}{\partial r}\right|_{\xi_i,\xi_j}=\sum_{p=0}^{N}u_{pj}\left.\frac{dh_p}{dr}\right|_{\xi_i}=\sum_p \underbrace{\hat{D}_{ip}u_{pj}}_{mxm}=:D_r\underline{u}$$

Matrix-free operator evaluation

diagonal mass matrix

$$D_r=(I\otimes I\otimes\hat{D}) \qquad G_{rs}=J\circ B\circ\left(\frac{\partial r}{\partial x}\frac{\partial s}{\partial x}+\frac{\partial r}{\partial y}\frac{\partial s}{\partial y}+\frac{\partial r}{\partial z}\frac{\partial s}{\partial z}\right)$$

Spectral element method

- Spectral element coefficients stored on element basis ($\underline{u}_L$ not $\underline{u}$)

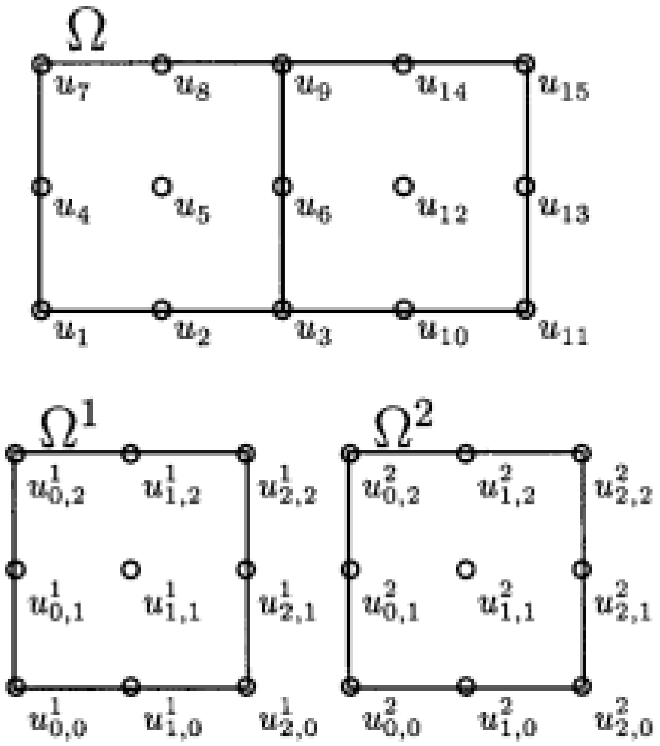
$$\underline{w} = A\underline{u} = Q^T A_L Q\underline{u}, \qquad \underline{w}_L := Q\underline{w}, \qquad \underline{u}_L := Q\underline{u}$$

$$\underline{w}_L = QQ^T A_L \underline{u}_L$$

local work (matrix-matrix products)

nearest-neighbor (gather-scatter) exchange

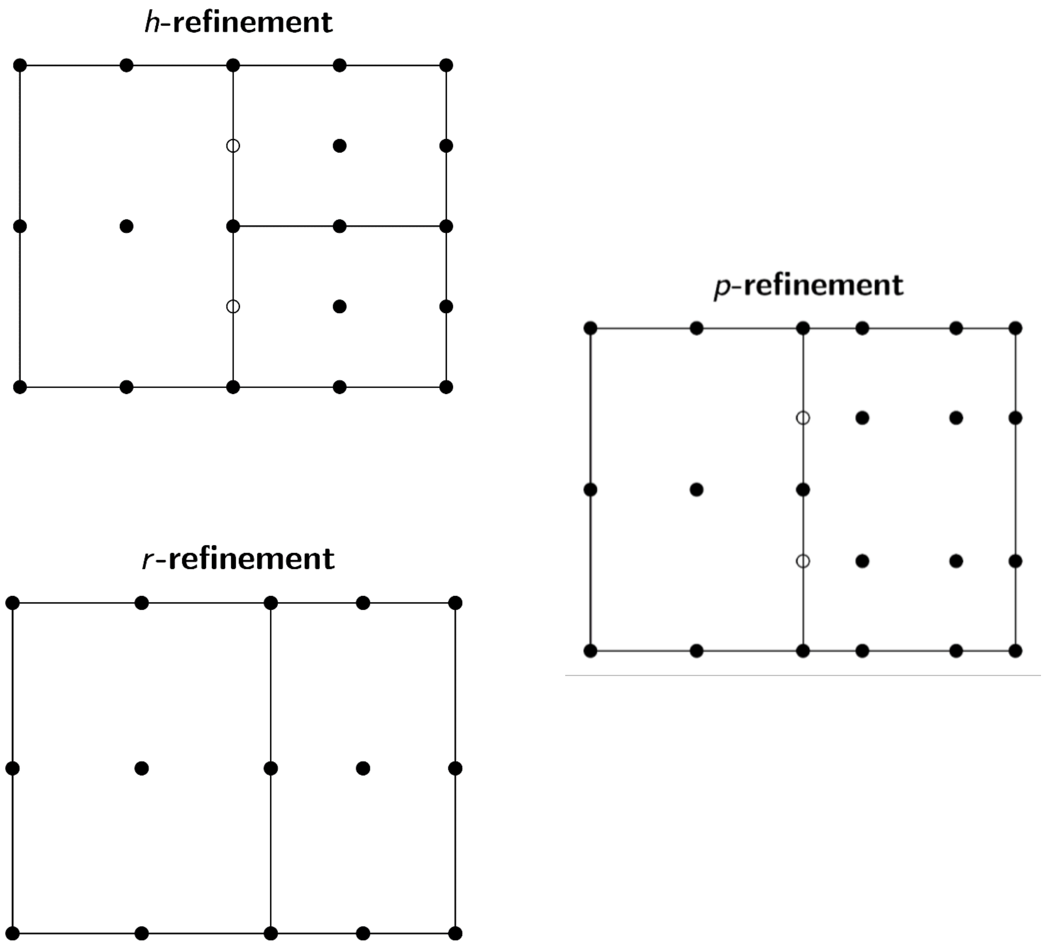
$$A_L := \begin{bmatrix} A^1 & & & \\ & A^2 & & \\ & & \ddots & \\ & & & A^E \end{bmatrix}$$



- Decouples complex physics (A_L) from communication (QQ^T)

Fischer at al 2002

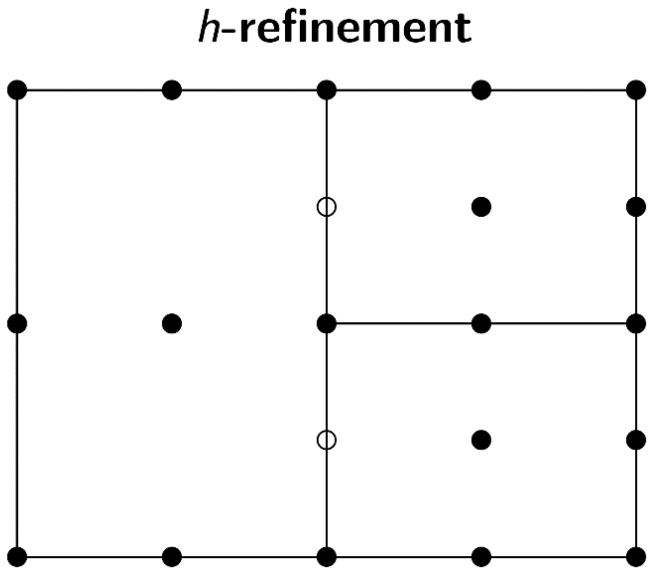
Adaptive mesh refinement



AMR approach:

- **h-refinement** - number of degrees of freedom modified by splitting/merging elements
- **p-refinement** - number of degrees of freedom modified by local variation of the polynomial order
- **r-refinement** – constant number of degrees of freedom; resolution modified by redistribution of grid points

Adaptive mesh refinement

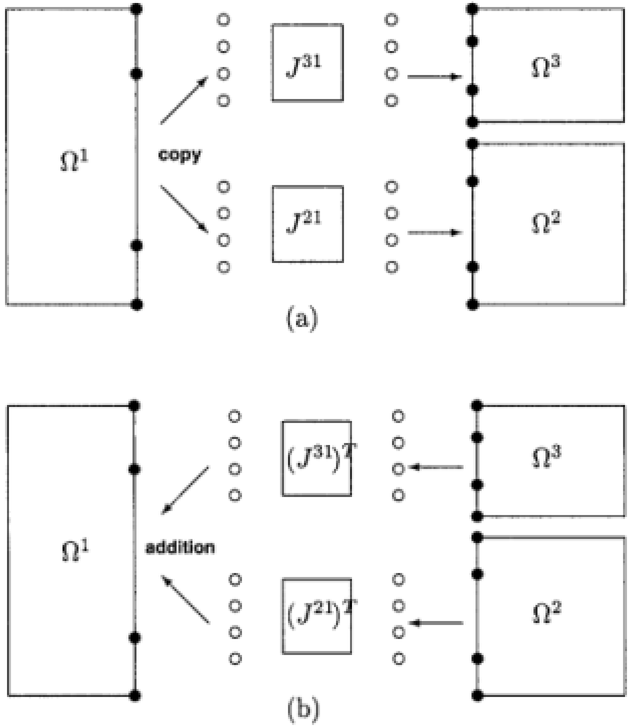


AMR approach:

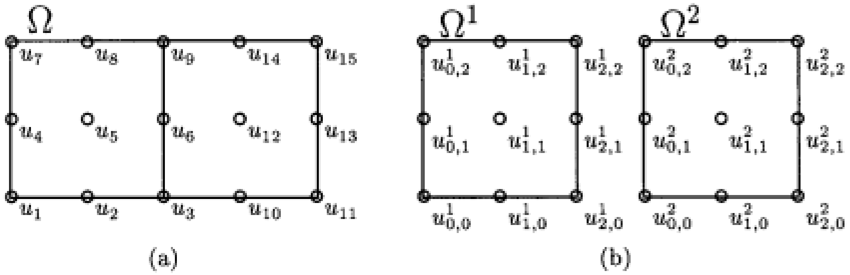
- **h-refinement** - number of degrees of freedom modified by splitting/merging elements

P. F. Fisher, G. W. Kruse, F. Loth, **Spectral element methods for transitional flows in complex geometries**, J. of Sci. Comput. 17 1, 81-98, 2002

Adaptive mesh refinement

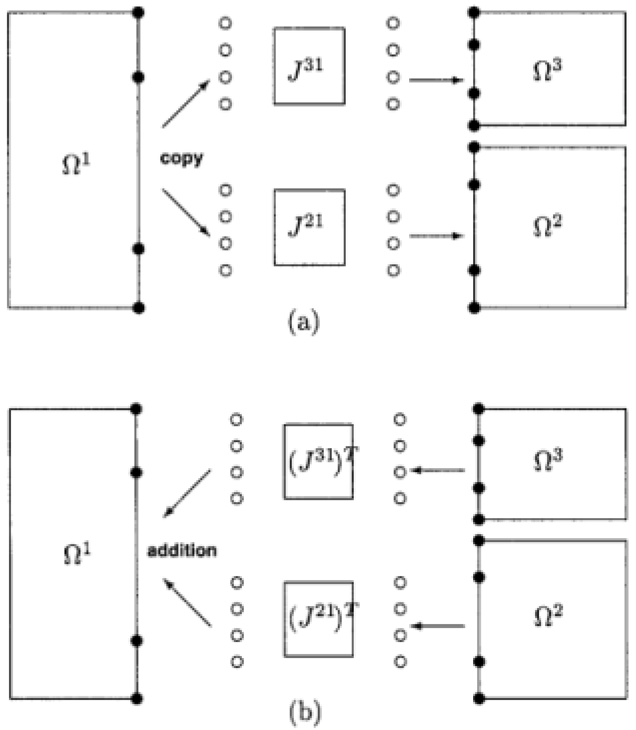


- **Geometrically nonconforming**
- **Parent-child communication** between elements requires additional interpolation operator J
- **Hanging nodes**: information required

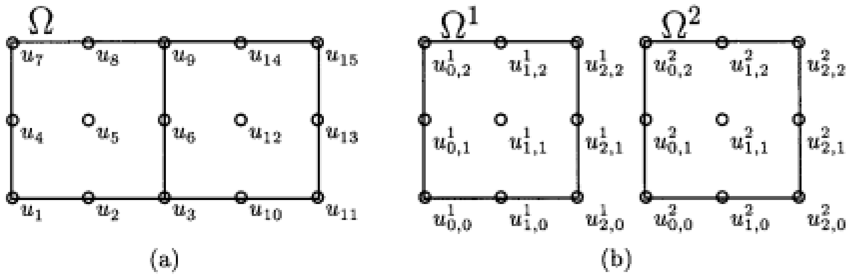


Fischer at al 2002

Adaptive mesh refinement



- **Functionally conforming**
- J – spectral interpolation
- Conforming vs. nonconforming matching condition on interface
- **Conforming-space/ nonconforming-mesh approach**



Fischer at al 2002

Adaptive mesh refinement

- Gather-scatter operator
  - Helmholtz equation
    $$J_L Q Q^T J_L^T$$
  - Pressure preconditioner
    $$J_L Q Q^T J_L^{-1}$$
- Mass matrix diagonalization
  $$\tilde{b} \coloneqq Q^T J_L^T B_L e_L$$
- Coarse grid operator
  $$\hat{A}_{ij} \coloneqq a_i^T A_L a_j$$

Interpolation operator

$$J_{ij} = h_j(\xi_i^{cp})$$

Inverse interpolation operator

$$(J^{-1})_{ij} = \\ = \begin{cases} h_j(\xi_i^{pc}) & , if\ \xi_j^p \in \partial\Omega^p \cap \partial\Omega^c \\ 0 & , \quad otherwise \end{cases}$$

Adaptive mesh refinement

- Gather-scatter operator
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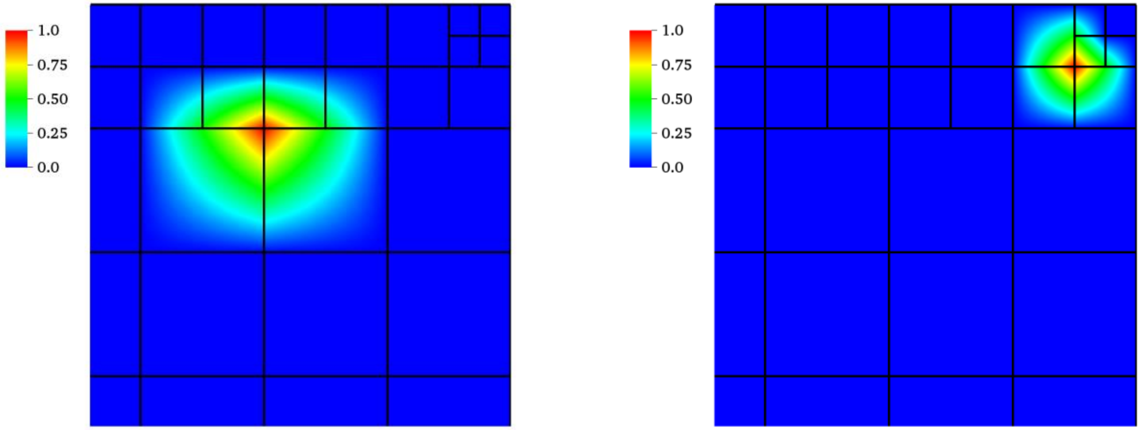
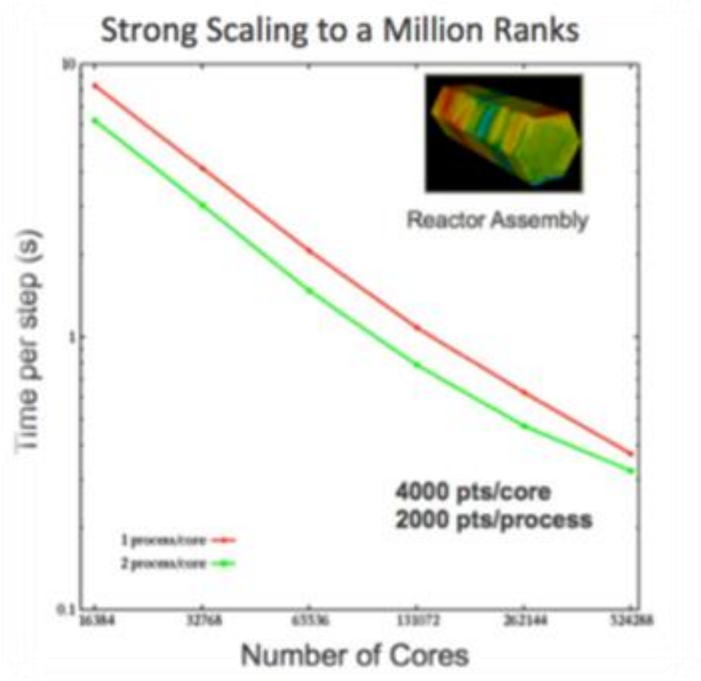


Examples of the base functions for coarse grid solver interpolation

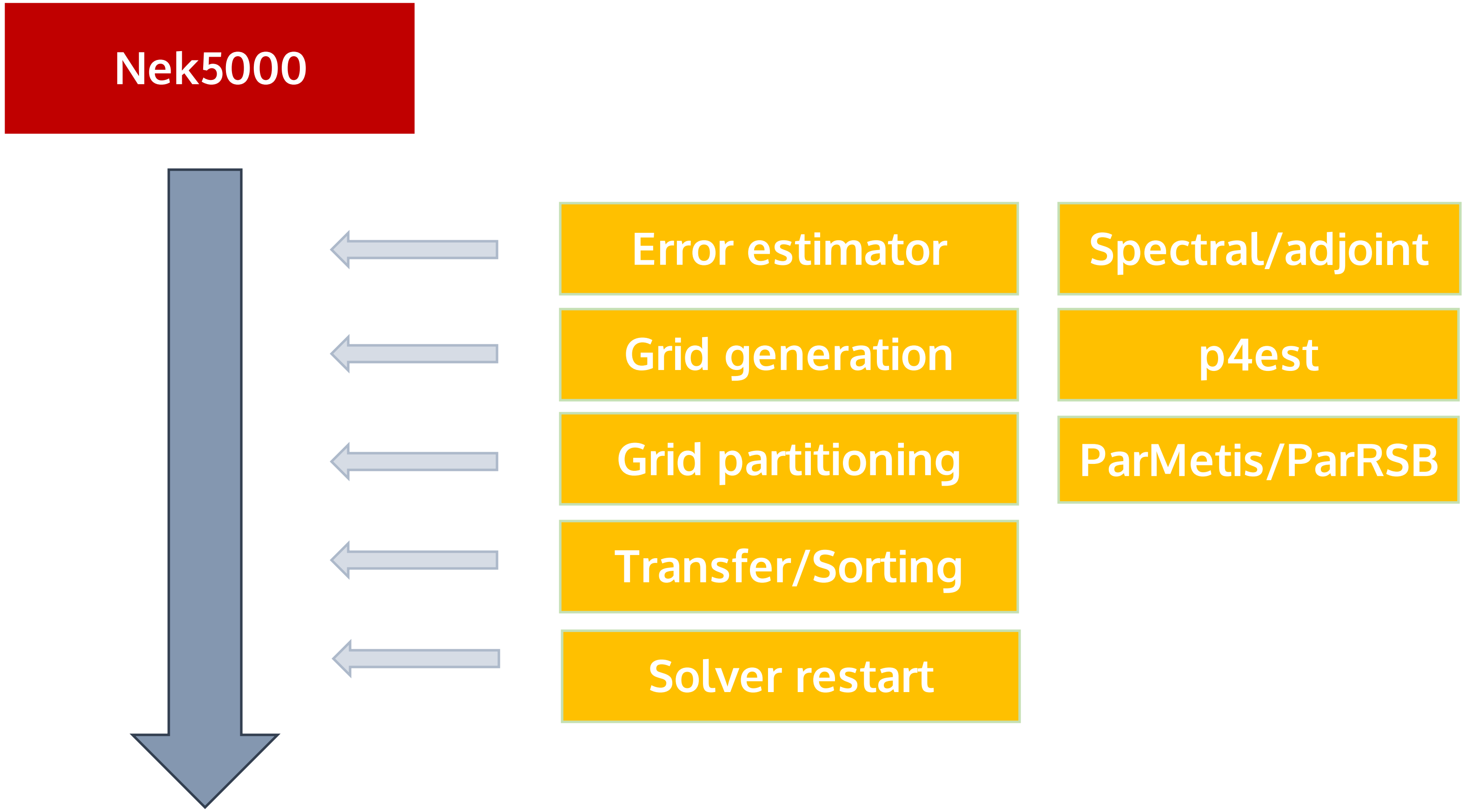
Nek5000 implementation



- bla>500k cores on ALCF BG/Q Mira
- Full scale parallel efficiency 0.6 with two processes per core

- General CFD solver:
  - incompressible and low Mach approximation
  - conjugate heat transfer
  - …
- Long development history
  - First commercially-available code for distributed memory computers
  - Gordon Bell Prize 1999
- Based on Spectral Element Method
  - High order discretisation
  - Low numerical diffusivity
  - Good scaling properties

Nek5000 implementation



Nek5000 implementation

Spectral error estimator

- Sum of the truncation error and the quadrature error
- Local calculation performed within single spectral element
- Based on variable expansion in Legendre base

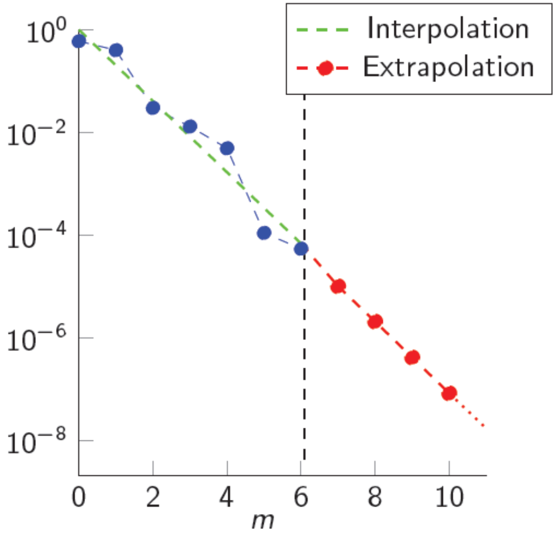
$$u_N^e(r) = \sum_{n=0}^{N} a_n^e L_n(r),$$

- Legendre coefficient approximation

$$a(n) = C\, e^{-\sigma n}$$

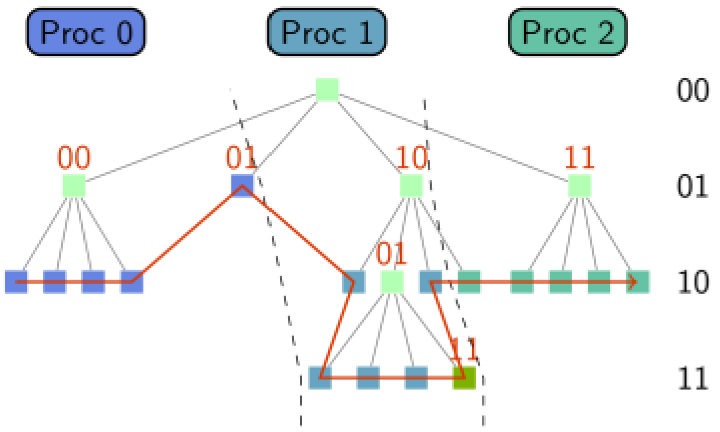
- Error estimate

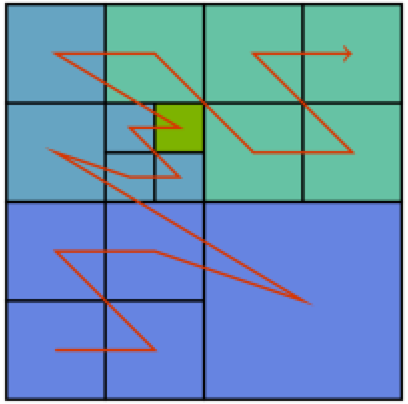
$$\epsilon_{est} = \left(\frac{2a_N^2}{2N+1} + \int_{N+1}^{\infty} \frac{2[a(n)]^2}{2n+1} dn \right)^{1/2}$$



Legendre coefficient

Nek5000 implementation



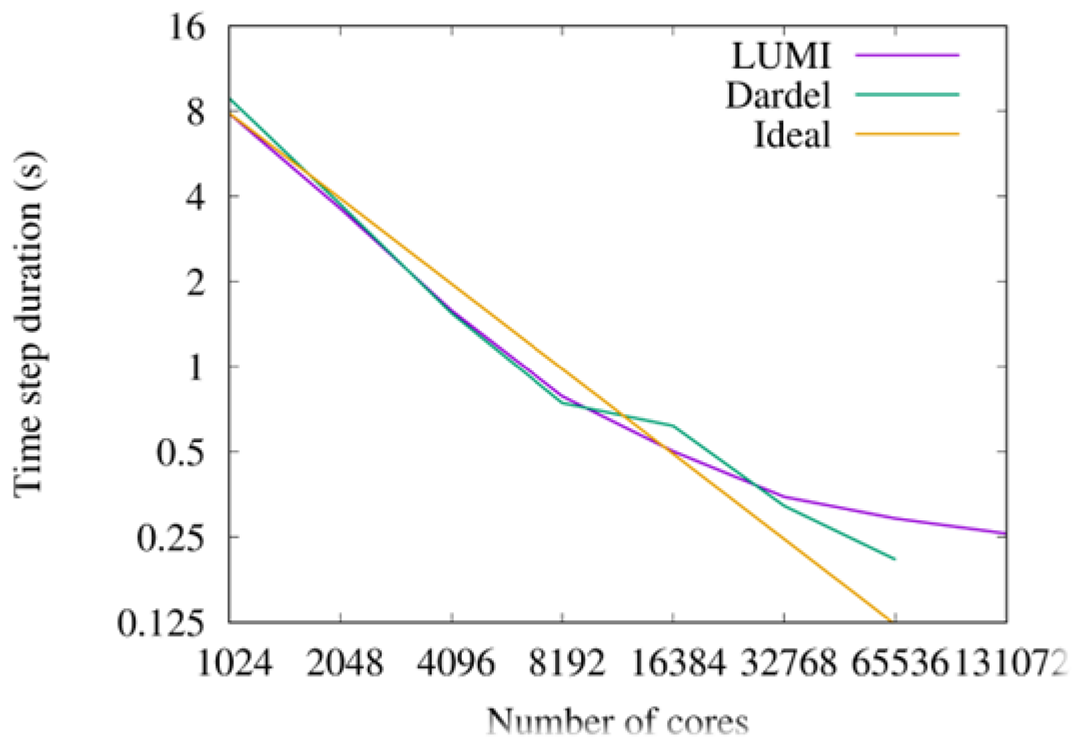


Burstedde, Wilcox, Ghattas, SISC, 2011

- p4est - AMR on forests of octrees
- Adaptive, **multi-block tree-code** to manage a quad- or octree of non-overlapping fixed sized grids
- Parallel, highly scalable on realistic applications; up to 220320 cores with parallel efficiency 70%
- **Refinement/coarsening performed locally**
- Element based with no geometrical restriction
- www.p4est.org
- C. Burstedde, L. Wilcox, and O. Ghattas. **p4est: Scalable algorithms for parallel adaptive mesh refinement on forests of octrees.** SIAM J. Sci. Comput., 33(3):1103–1133, 2011

Nek5000 implementation

Strong scaling on Dardel and LUMI

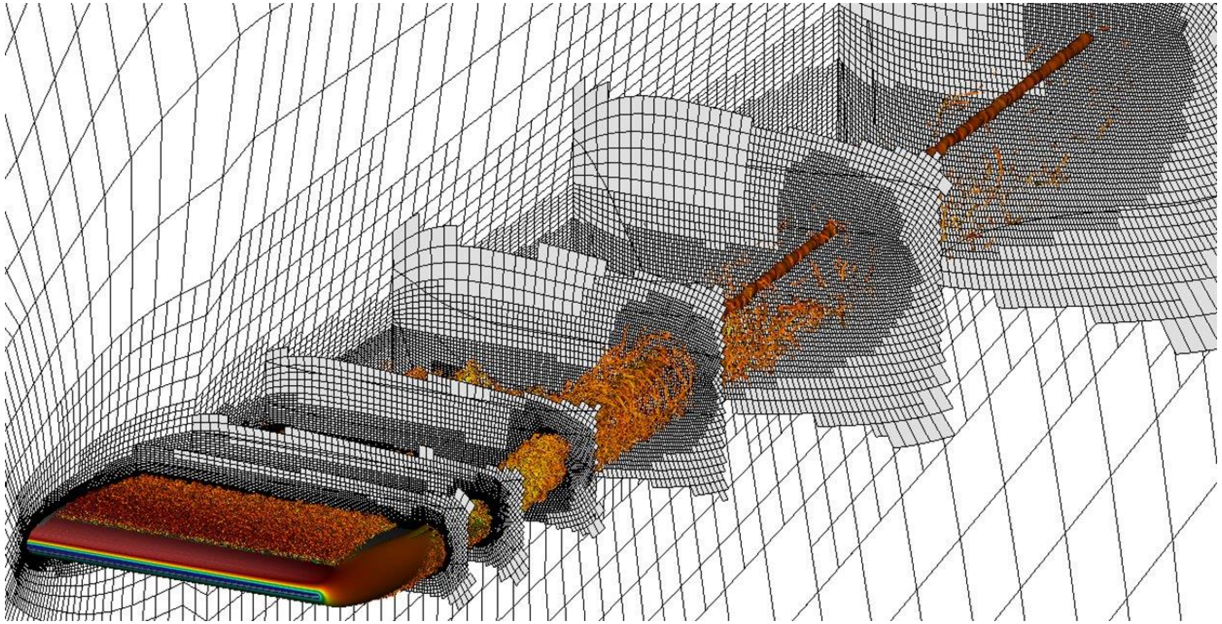


Performance of AMR run:

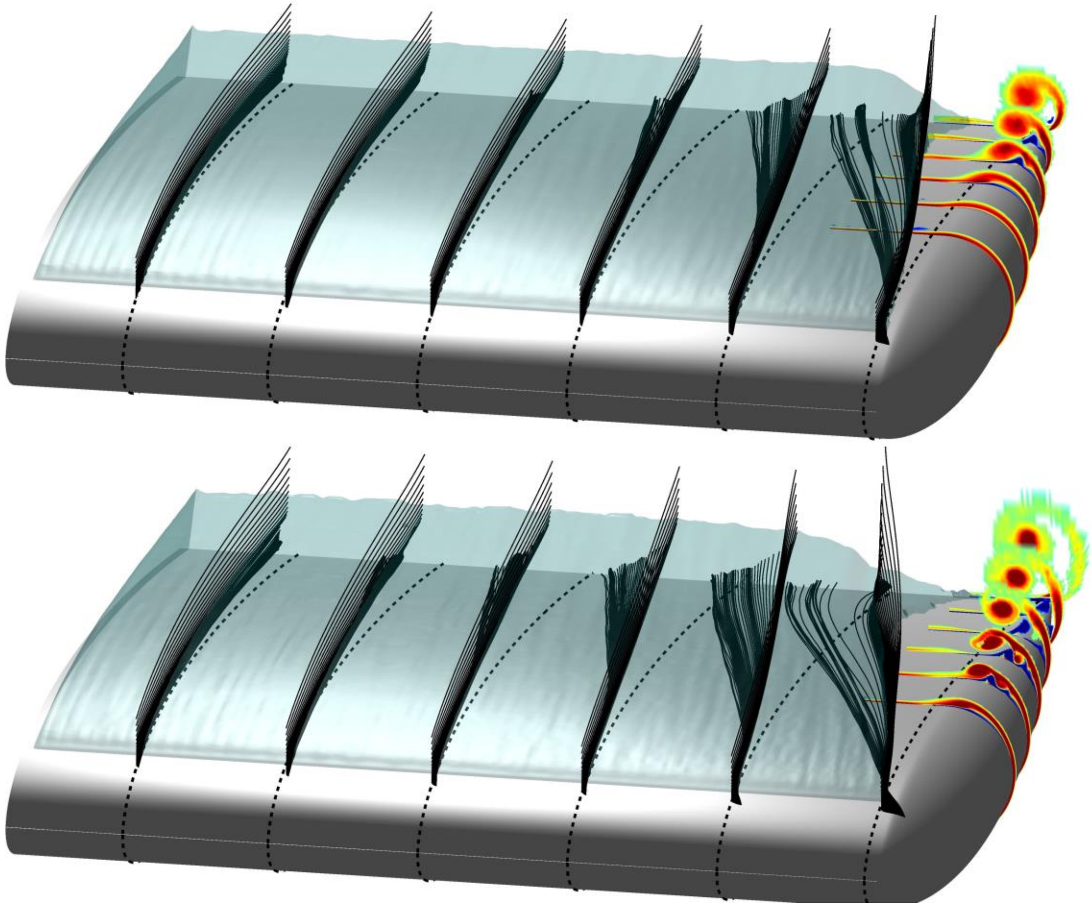
- 1024 cores
- Global element number (21 ref.)
  - Initial 113952
  - Final 131781
- Total simulation time 85242 sec
- **Total AMR time 1269 sec (1.5%)**
- Percentage of different operations (AMR – 100%):
  - I/O 5.1%
  - Error estimate 13.7%
  - Mesh regeneration 0.3%
  - Data transfer 0.5%
  - Solver restart 77.0%

NACA0012 airfoil with rounded tip

Mesh structure and vortical flow features

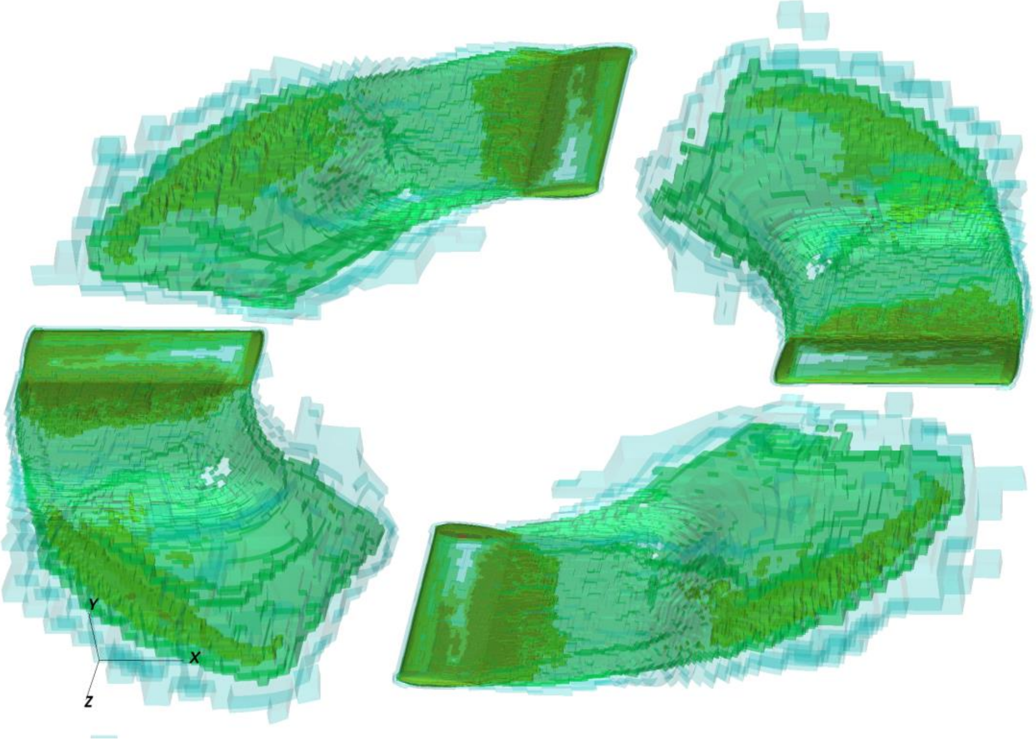


Flow lines of an averaged velocity field and position of a tip vortex

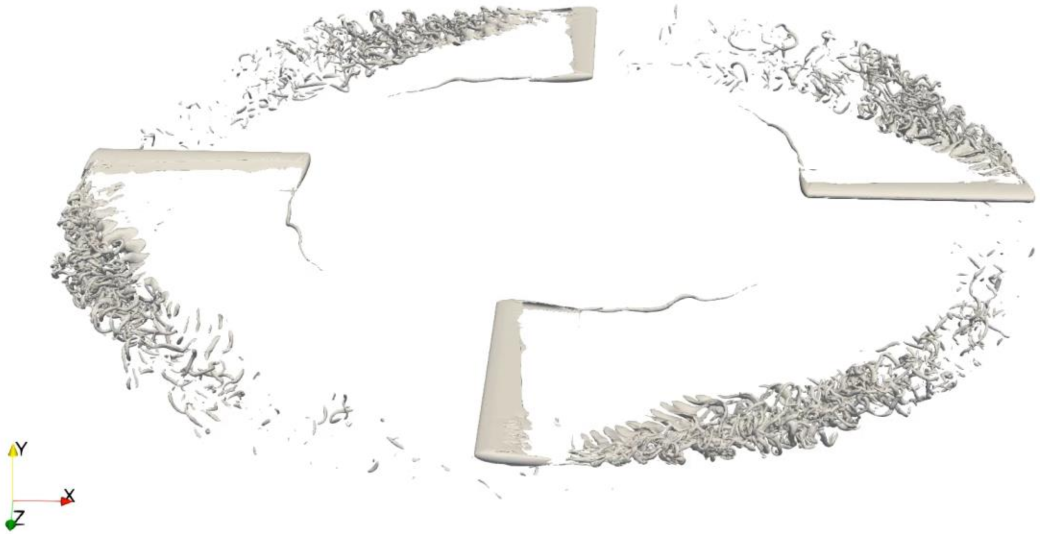


A simplified rotor with four blades

Domain regions covered by different refinement levels



Vortical structures

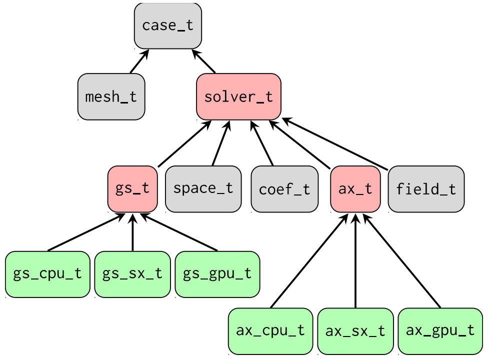


Current work on Neko

- High-order spectral element flow solver
  - Incompressible Navier-Stokes equations
  - Matrix-free formulation, **small tensor products**
  - **Gather-scatter** operations between elements
- Modern **object-oriented** approach (Fortran 2008)

```fortran
! Base type for a matrix-vector product providing Ax
type, abstract :: ax_t
  contains
    procedure(ax_compute), nopass, deferred :: compute
end type ax_t

! Abstract interface for computing Ax
abstract interface
   subroutine ax_compute(w, u, coef, msh, Xh)
     implicit none
     type(space_t), intent(inout) :: Xh
     type(mesh_t),  intent(inout) :: msh
     type(coef_t),  intent(inout) :: coef
     real(kind=dp), intent(inout) :: w(:,:,:,:)
     real(kind=dp), intent(inout) :: u(:,:,:,:)
   end subroutine ax_compute
end interface
```

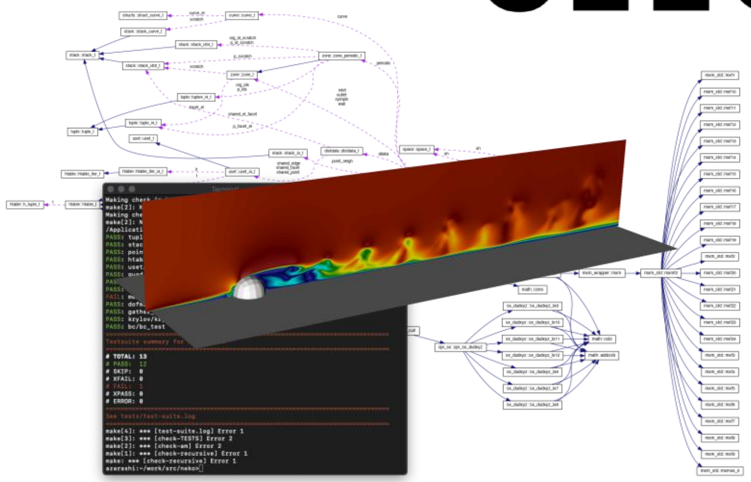


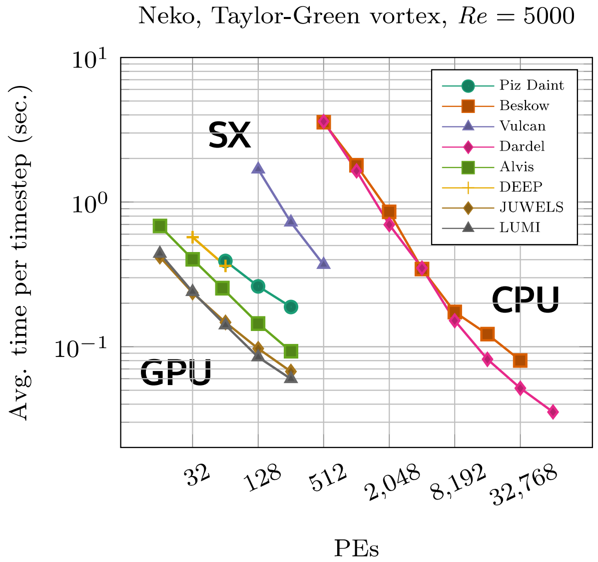
- Various hardware-backends
  - CPUs, GPUs down to exotic vector processors and FPGAs
    - **Device abstraction layer** for accelerators (CUDA/HIP/OpenCL)
- Modern Software Engineering (pFUnit, ReFrame, **Spack**)

> spack install neko+cuda

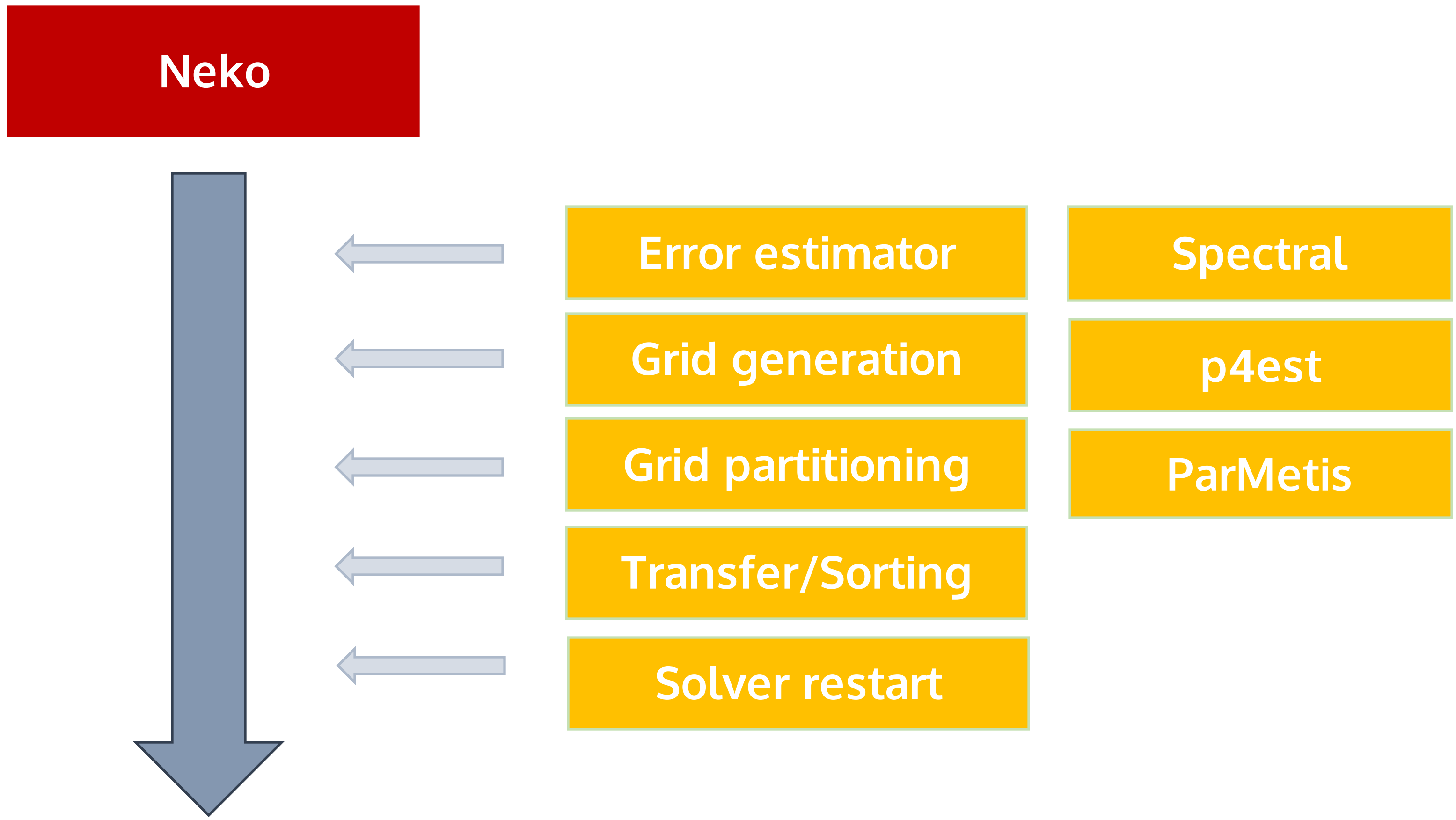
> spack install neko+cuda

ExtremeFLOW/neko

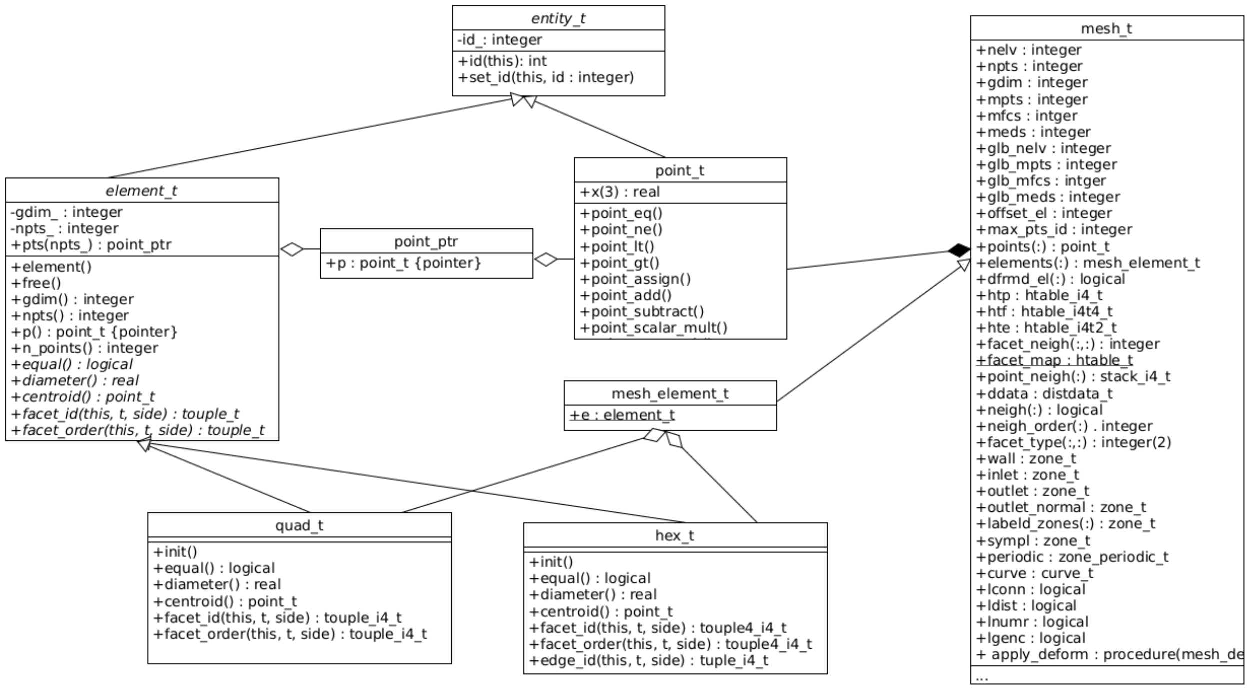




Current work on Neko



Current work on Neko

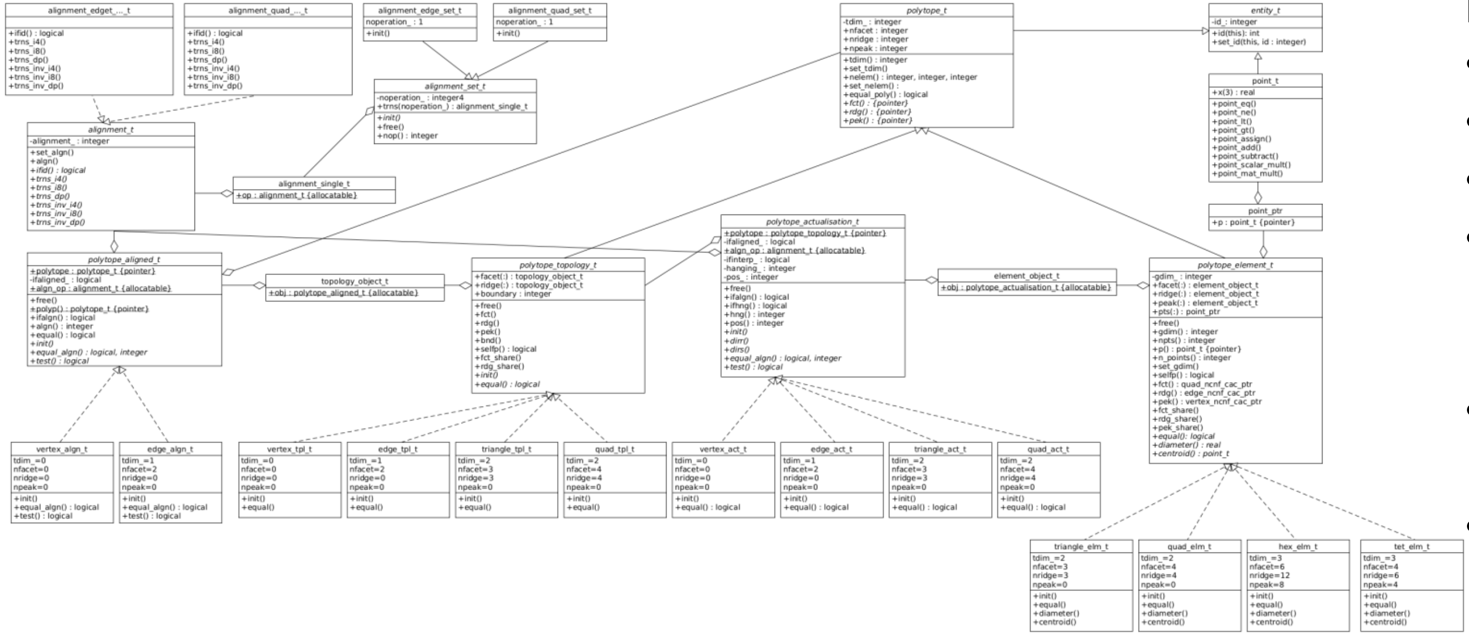


Class diagram for mesh type

Mesh description:

- Compact and flexible
- Well suits conforming meshes
- Combines topology and geometry
- Connectivity defined by global id of a physical point
  - No easy way to describe hanging nodes (element local perspective needed)
- Straightforward to import conforming p4est data, but problem with nonconforming meshes

Current work on Neko



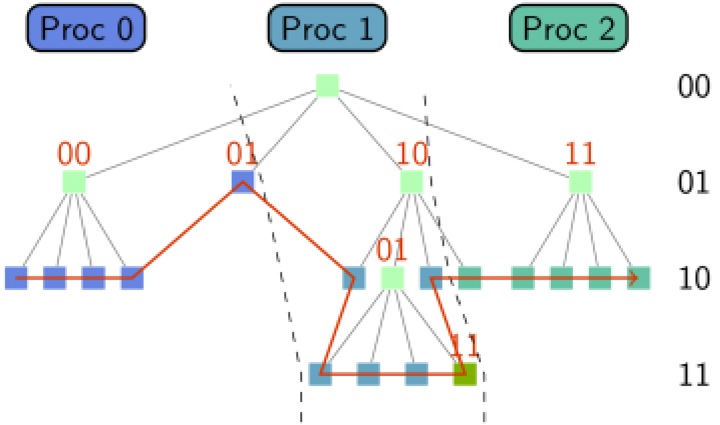
Class diagram for mesh type

New mesh description:

- Flexible, but complex
- Supports nonconforming meshes
- Splits topology and geometry
- Distinguishes abstract object and its realisation (element local perspective)
- Straightforward to import nonconforming p4est data
- Under construction

Current work on Neko

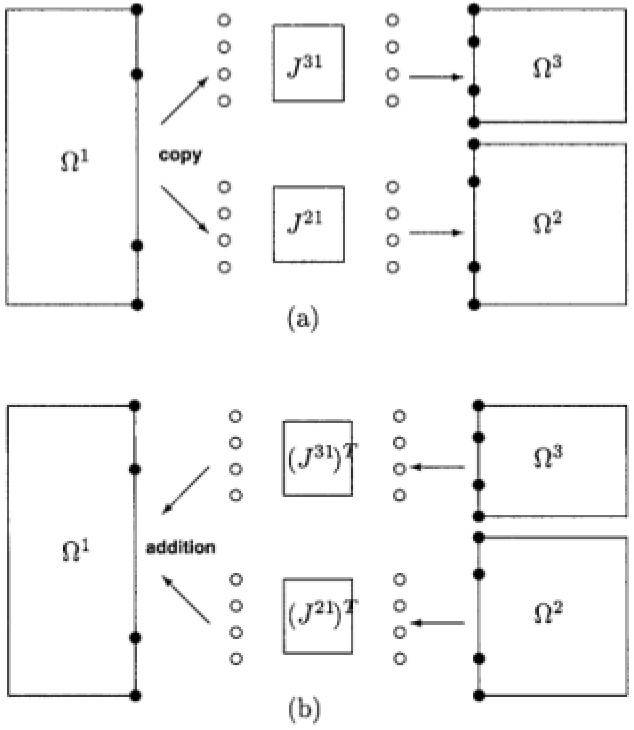
AMR workflow:
- Collect error indicator on GPU
- Perform refinement and mesh reconstruction on CPU
- Reconstruct simulation variables on GPU
- Restart the solver



Schematic representation of element distribution among MPI ranks.
Burstedde, Wilcox, Ghattas, SISC, 2011

Main challenges:
- Interpolation operator for direct stiffness summation
  - Frequent, performed on GPU
  - Interpolation operator acting on a small amount of element faces and edges
  - Four different 2D operators for faces and two 1D operators for edges
- Reconstruction of the simulation variables
  - Rare, performed on GPU
  - 3D interpolation operator acting on a small amount of elements
  - Requires communication
  - Three steps: refinement, global redistribution, coarsening
- Solver restart

Current work on Neko

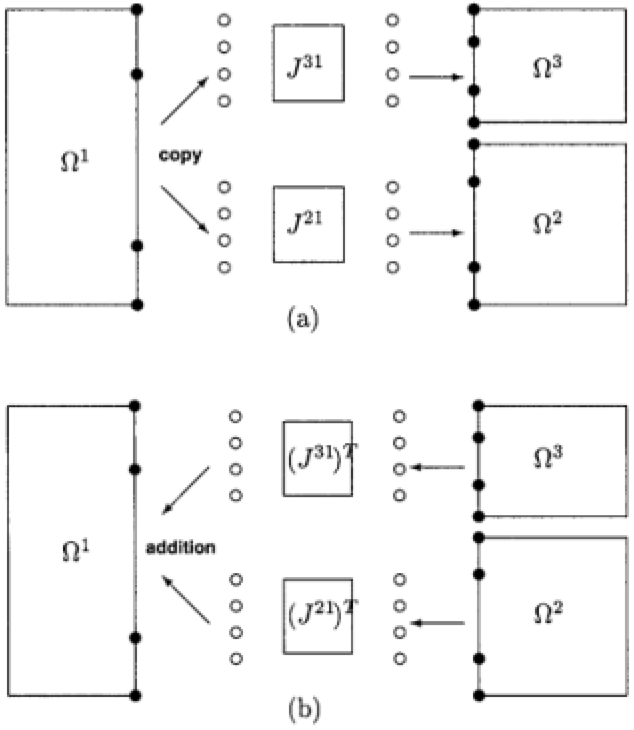


Data exchange at nonconforming interface
Fischer at al 2002

Communication kernels refactoring:

- Direct stiffness summation based on a single point information
- Nonconforming solver introduces interpolation operator acting on objects (element faces and edges)
- Challenging on GPUs as interpolation operator acts on a small data sets randomly distributed in a big array
- Work imbalance in the interpolation operator

Current work on Neko



Data exchange at nonconforming interface
Fischer at al 2002

- Data for interpolation operation not contiguous and randomly ordered
- Performance will be dominated by memory latency
  - Necessary to have as many as possible memory operations overlapping to get maximum memory bandwidth
- Possible ways for data exchange:
  - Keep high point multiplicity and treat nonconforming interfaces separately
  - Lower face multiplicity by separately numbering each of the children faces

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