# Driving metric mesh adaptivity in a nonlinear minimization scheme

Iztok Bajc, Frédéric Hecht, Slobodan Žumer

Univerza v Ljubljani



Fakulteta za matematiko in fiziko Univerza v Ljubljani Slovenija



Laboratoire Jacques-Louis Lions Université Pierre et Marie Curie Paris 6, France



Inštitut Jožef Stefan Ljubljana Slovenija

### **Motivations:**

• Tendence to make simulations more and more realistic.

- Tendence to make simulations more and more **realistic**.
- Nonlinear problems increasingly important.

- Tendence to make simulations more and more **realistic**.
- Nonlinear problems increasingly important.
- In general not easy to solve. Iterative methods needed.

- Tendence to make simulations more and more **realistic**.
- Nonlinear problems increasingly important.
- In general not easy to solve. Iterative methods needed.
- If we use **finite elements**:

- Tendence to make simulations more and more **realistic**.
- Nonlinear problems increasingly important.
- In general not easy to solve. Iterative methods needed.
- If we use **finite elements**:
  - > large problems

- Tendence to make simulations more and more **realistic**.
- Nonlinear problems increasingly important.
- In general not easy to solve. Iterative methods needed.
- If we use **finite elements**:
  - > large problems
  - > unknown proceeding of iterates in configuration space

#### **Motivations:**

- Tendence to make simulations more and more **realistic**.
- Nonlinear problems increasingly important.
- In general not easy to solve. Iterative methods needed.
- If we use **finite elements**:
  - > large problems
  - unknown proceeding of iterates in configuration space

Mesh adaptivity

welcome

#### **Motivations:**

- Tendence to make simulations more and more **realistic**.
- Nonlinear problems increasingly important.
- In general not easy to solve. Iterative methods needed.
- If we use finite elements:
  - > large problems
  - unknown proceeding of iterates in configuration space
  - » spatially unpredictable and perhaps very small details

Mesh adaptivity

welcome

#### **Motivations:**

- Tendence to make simulations more and more realistic.
- Nonlinear problems increasingly important.
- In general not easy to solve. Iterative methods needed.
- If we use finite elements:
  - > large problems
  - unknown proceeding of iterates in configuration space
  - » spatially unpredictable and perhaps very small details

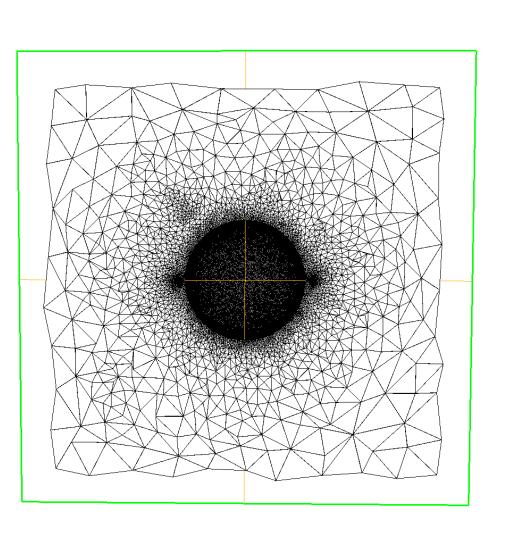
### Mesh adaptivity

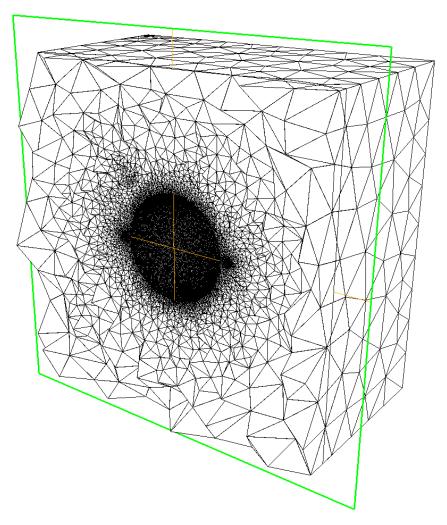
<u>welcome</u>

or even

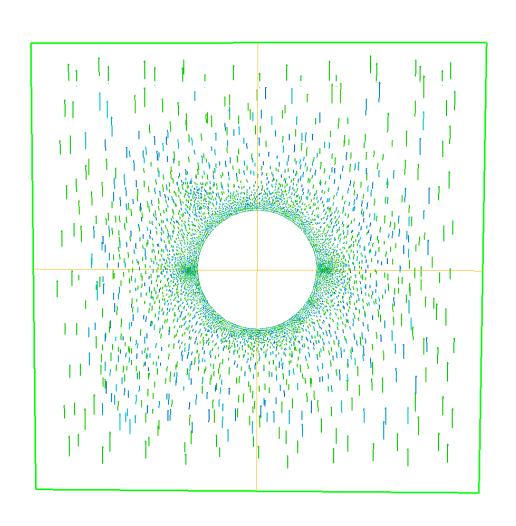
<u>required</u>

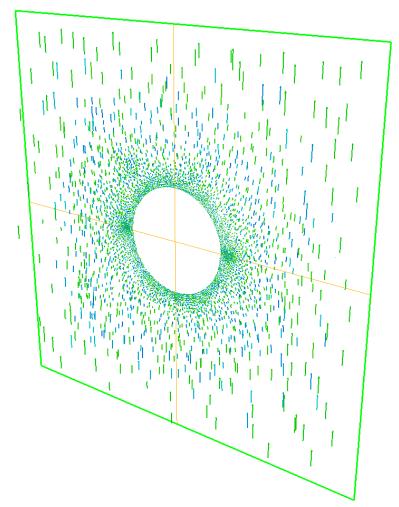
# Example – confined liquid crystals



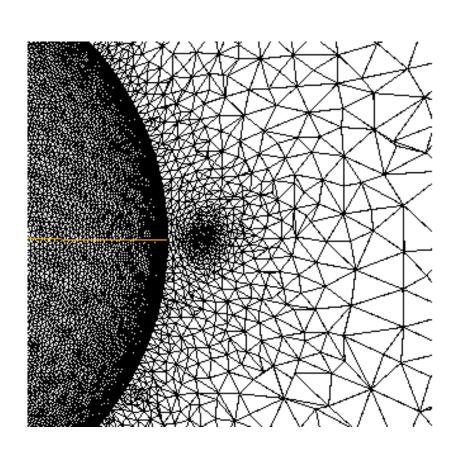


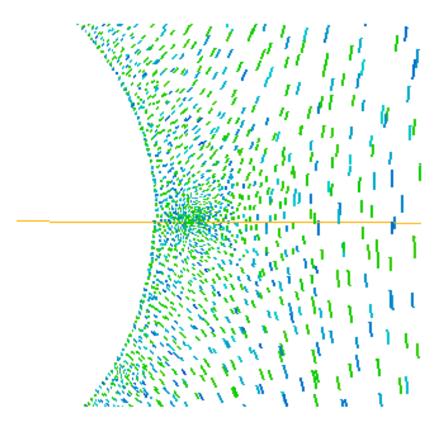
# Example – confined liquid crystals





## **Example – confined liquid crystals**





$$F(Q)$$
 min:

$$\delta F(Q) = F'(Q)\delta Q = 0$$

Euler-Lagrange equations

$$F(Q)$$
 min:

$$\delta F(Q) = F'(Q)\delta Q = 0$$

**Euler-Lagrange equations** 

$$\begin{split} \delta F(Q) &= \delta \int_{\Omega} f(Q, \nabla Q) dV \\ &= \int_{\Omega} \left( \frac{\partial f}{\partial Q} - \frac{\partial}{\partial r} \frac{\partial f}{\partial (\nabla Q)} \right) \delta Q dV + \int_{\partial \Omega} \frac{\partial f}{\partial (\nabla Q)} \cdot \nabla \delta Q dV \\ &= \int_{\Omega} L \nabla Q_{ij} \cdot \nabla \varphi_{ij} + \left( A Q_{ij} + B Q_{ik} Q_{kj} + C Q_{ik} Q_{kl} Q_{lj} \right) \varphi_{ij} dV - W \int_{\partial \Omega} \left( Q_{ij} - Q_{ij}^{\ 0} \right) \varphi_{ij} dA \end{split}$$

$$F(Q)$$
 min:  $\delta F(Q) = F'(Q)\delta Q = 0$  Euler-Lagrange equations

$$\begin{split} \delta F(Q) &= \delta \int_{\Omega} f(Q, \nabla Q) dV \\ &= \int_{\Omega} \left( \frac{\partial f}{\partial Q} - \frac{\partial}{\partial r} \frac{\partial f}{\partial (\nabla Q)} \right) \delta Q dV + \int_{\partial \Omega} \frac{\partial f}{\partial (\nabla Q)} \cdot \overset{\square}{v} \delta Q dV \\ &= \int_{\Omega} L \nabla Q_{ij} \cdot \nabla \varphi_{ij} + \left( A Q_{ij} + B Q_{ik} Q_{kj} + C Q_{ik} Q_{kl} Q_{lj} \right) \varphi_{ij} dV - W \int_{\partial \Omega} \left( Q_{ij} - Q_{ij}^{\ 0} \right) \varphi_{ij} dA \end{split}$$

$$F(Q)$$
 min:

$$\delta F(Q) = F'(Q)\delta Q = 0$$

**Euler-Lagrange equations** 

$$\delta F(Q) = \delta \int_{\Omega} f(Q, \nabla Q) dV$$

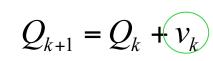
$$= \int_{\Omega} \left( \frac{\partial f}{\partial Q} - \frac{\partial}{\partial r} \frac{\partial f}{\partial (\nabla Q)} \right) \delta Q dV + \int_{\partial \Omega} \frac{\partial f}{\partial (\nabla Q)} \cdot \overset{\square}{V} \delta Q dV$$

$$= \int_{\Omega} L \nabla Q_{ij} \cdot \nabla \varphi_{ij} + \left( A Q_{ij} + B Q_{ik} Q_{kj} + C Q_{ik} Q_{kl} Q_{lj} \right) \varphi_{ij} dV - W \int_{\Omega} \left( Q_{ij} - Q_{ij}^{\ 0} \right) \varphi_{ij} dA$$

$$F''(Q_k) \widehat{v_k} \varphi = -F'(Q_k) \varphi$$

 $(\varphi - test functions)$ 

Newton iteration equation



(next iteration step)

Two tasks:

#### Two tasks:

> Coupling: mesh adaptivity + nonlinear minimization.

#### Two tasks:

- > Coupling: mesh adaptivity + nonlinear minimization.
- > Role played by various **parameters**.

#### Two tasks:

- > Coupling: mesh adaptivity + nonlinear minimization.
- > Role played by various parameters.

• Not much adressed until now [1].

<sup>[1]</sup> I. Danaila, F. Hecht, *A finite element method with mesh adaptivity for computing vortex states in fast-rotating Bose-Einstein condensates.* Jour. of Computat. Phys., **229** (2010) 6946-6960.

#### Two tasks:

- > Coupling: mesh adaptivity + nonlinear minimization.
- > Role played by various **parameters**.

- Not much adressed until now [1].
- In particular not for **metric** mesh adaptivity.

<sup>[1]</sup> I. Danaila, F. Hecht, *A finite element method with mesh adaptivity for computing vortex states in fast-rotating Bose-Einstein condensates.* Jour. of Computat. Phys., **229** (2010) 6946-6960.

#### Two tasks:

- > Coupling: mesh adaptivity + nonlinear minimization.
- > Role played by various **parameters**.

- Not much adressed until now [1].
- In particular not for **metric** mesh adaptivity.
- Surely **not completely clarified**.

<sup>[1]</sup> I. Danaila, F. Hecht, A finite element method with mesh adaptivity for computing vortex states in fast-rotating Bose-Einstein condensates. Jour. of Computat. Phys., **229** (2010) 6946-6960.

# Metric mesh adaptivity in 3D

**Tools:** 

**Parameters** 

mshmet:

calculates metric

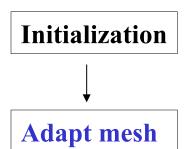
scFields, hmin, hmax, errm

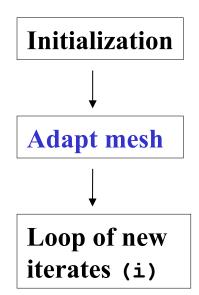
mmg3d:

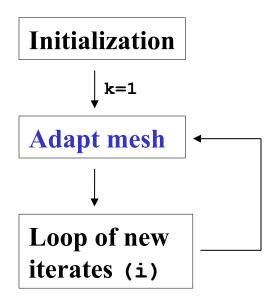
with this metric remeshes previous mesh

metric M, hmin, hmax, errm, hgrad

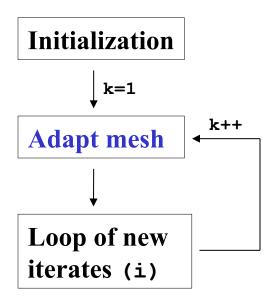
Initialization



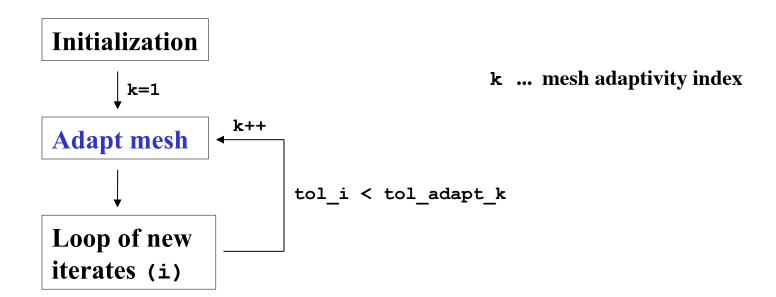


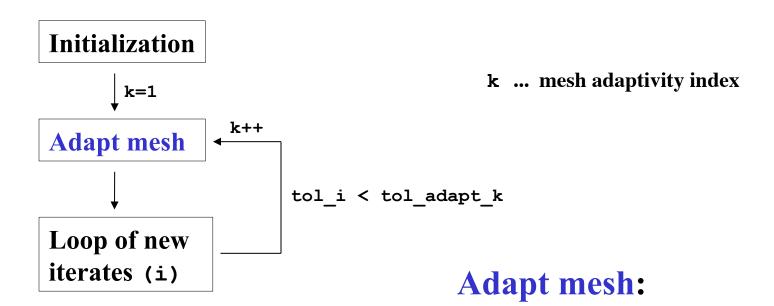


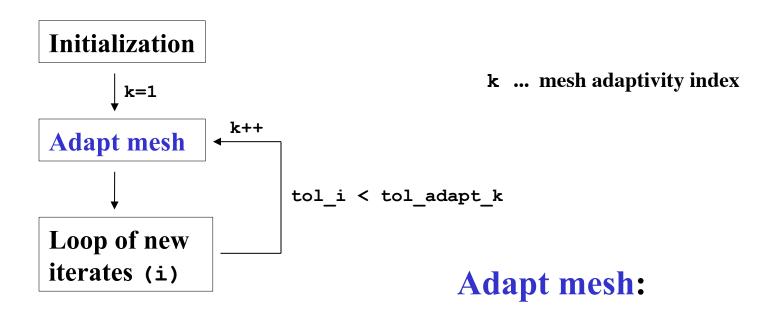
k ... mesh adaptivity index



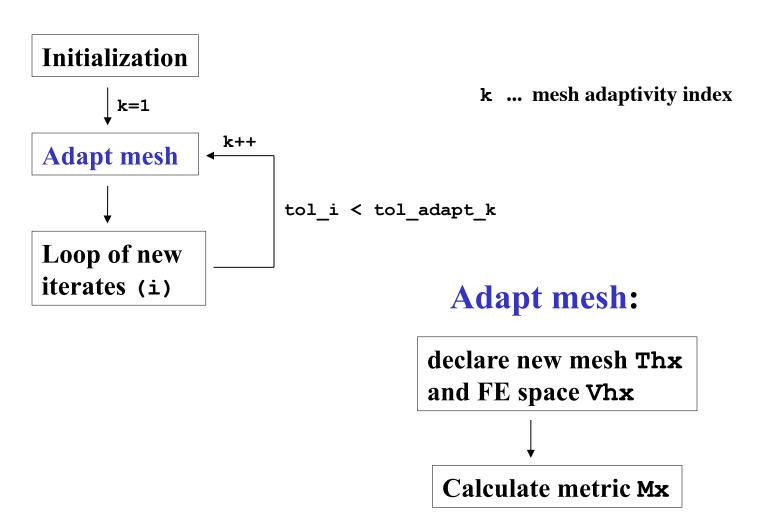
k ... mesh adaptivity index

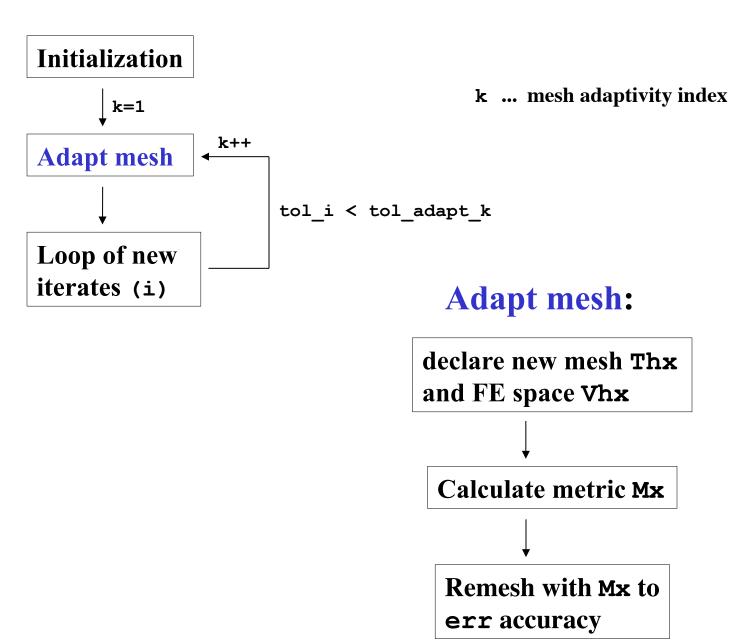


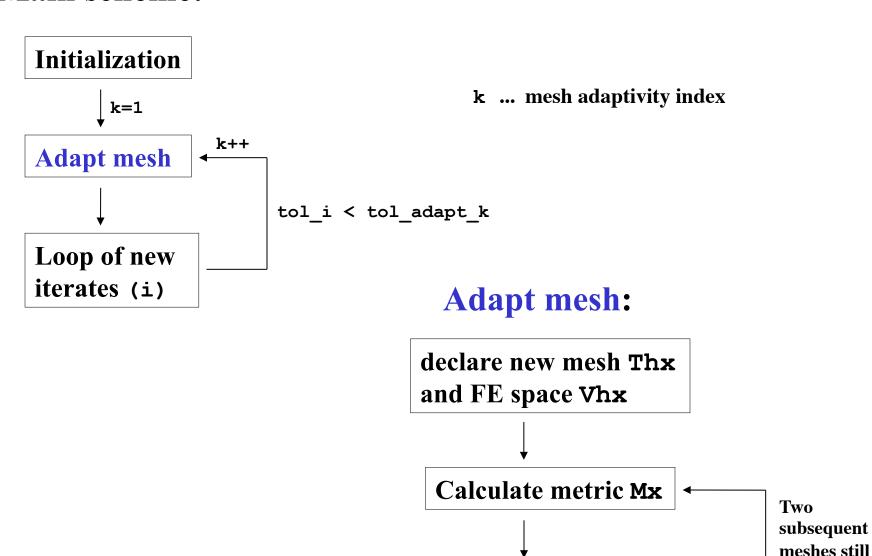




declare new mesh Thx and FE space Vhx



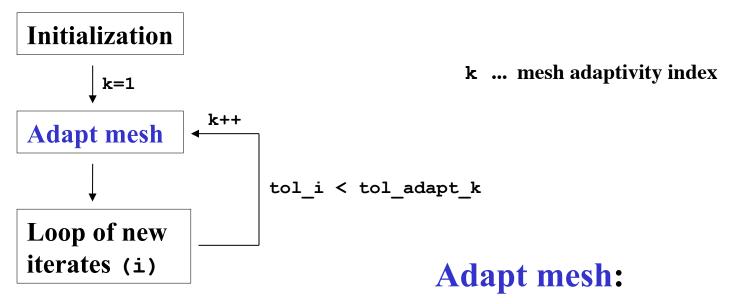




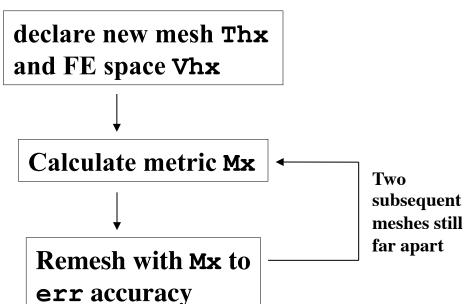
Remesh with Mx to

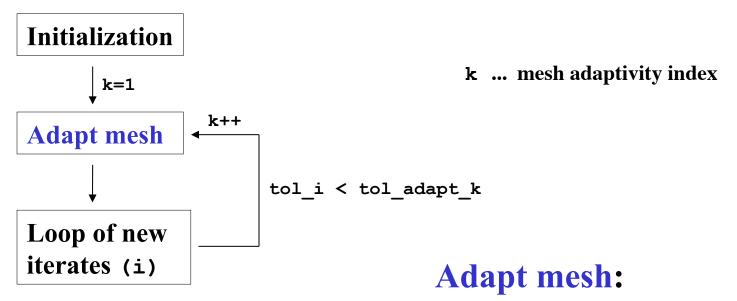
err accuracy

far apart



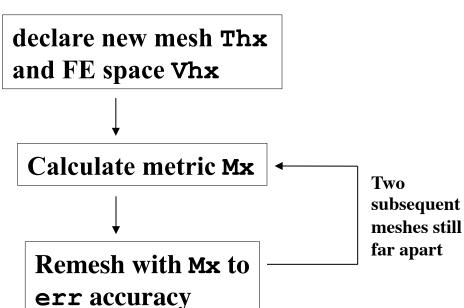
#### **Questions:**

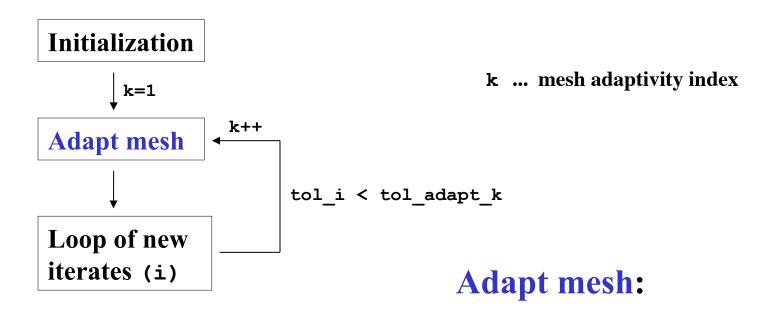




#### **Questions:**

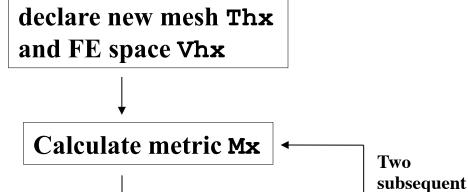
1) How many mesh adaptations to do?





#### **Questions:**

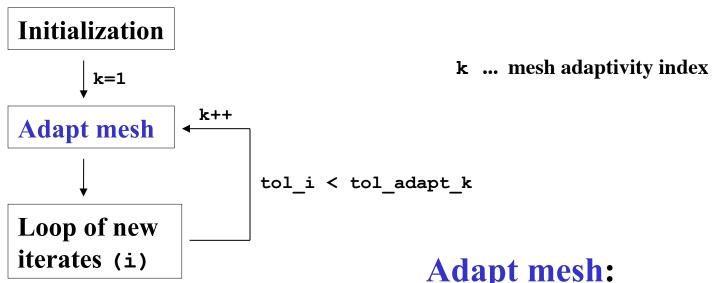
- 1) How many mesh adaptations to do?
- 2) At what **tolerances** to trigger new mesh adaptivity?



Remesh with Mx to

err accuracy

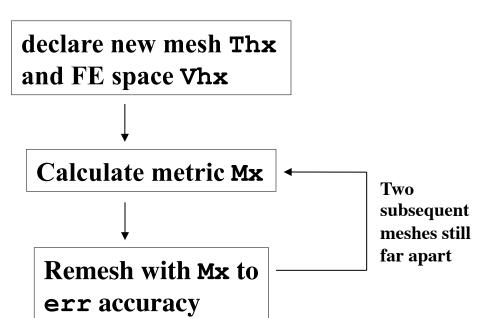
meshes still far apart

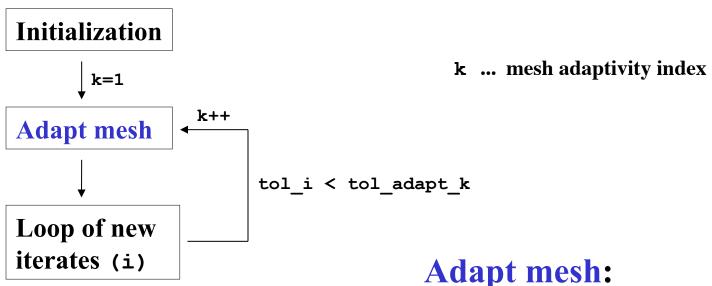


#### **Questions:**

- 1) **How many** mesh adaptations to do?
- 2) At what **tolerances** to trigger new mesh adaptivity?
- 3) To what **accuracy** compute new meshes?

### Adapt mesh:

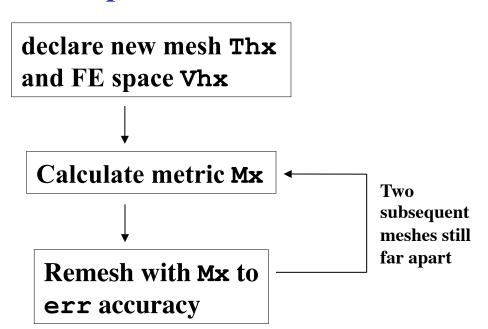




#### **Questions:**

- 1) **How many** mesh adaptations to do?
- 2) At what **tolerances** to trigger new mesh adaptivity?
- 3) To what **accuracy** compute new meshes?

Three (sets of ) free parameters!



1) Use a **fixed** nb of mesh adaptations.

- 1) Use a **fixed** nb of mesh adaptations.
- 2) Trigger new mesh adaptivity at a predefined, **fixed sequences of tolerances**.

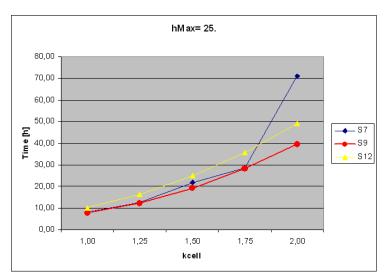
- 1) Use a **fixed** nb of mesh adaptations.
- 2) Trigger new mesh adaptivity at a predefined, **fixed sequences of tolerances**.
- 3) Compute new meshes at predefined, **fixed sequences of accuracies**.

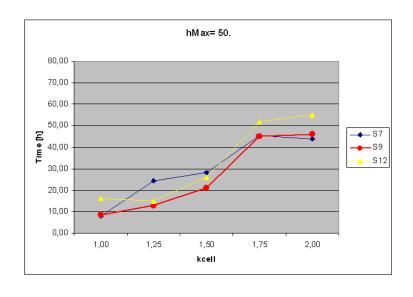
- 1) Use a **fixed** nb of mesh adaptations.
- 2) Trigger new mesh adaptivity at a predefined, **fixed sequences of tolerances**.
- 3) Compute new meshes at predefined, **fixed sequences of accuracies**.

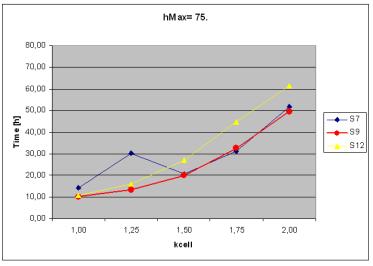
**Table 1.**Three sequences (arrays) used in calculations:

Mesh adaptation	S7 tolAdapt	errm	S9 tolAdapt	errm	S12 tolAdapt	errm
0. 1. 2.	0.5e-4 0.5e-3 0.5e-3	0.020 0.020 0.015	0.5e-4 0.5e-3 0.5e-3	0.020 0.020 0.015	0.5e-4 0.5e-3 0.5e-3	0.020 0.020 0.015
3. 4. 5.	0.5e-4 0.5e-5 0.5e-5	0.015 0.015 0.010	1.0e-4 1.0e-4 0.5e-4	0.020 0.015 0.015	1.0e-4 1.0e-4 0.5e-4	0.020 0.015 0.020
6. 7. 8. <b>9</b> .	1.0e-6 1.0e-6	0.015	1.0e-5 0.5e-5 0.5e-5 1.0e-6	0.015 0.015 0.010 0.010	0.5e-4 1.0e-5 1.0e-5 0.5e-5	0.015 0.015 0.015 0.015
10. 11. <b>12</b> .			1.0e-0	0.010	0.5e-5 0.5e-5 1.0e-6 1.0e-6	0.013 0.010 0.015 0.010

# Results and conclusions







ninax-25				
kcell/seq	<b>S</b> 7	S9	S12	
1,00	8,17	7,83	10,08	
1,25	12,42	12,33	16,25	
1,50	21,75	19,25	25,00	
1,75	28,50	28,17	35,67	
2,00	71,00	39,50	49,08	

nmax=50				
kcell/seq	S7 S9		S12	
1,00	8,00	8,50	16,00	
1,25	24,37	13,00	15,00	
1,50	28,00	21,00	26,00	
1,75	45,33	45,12	51,88	
2,00	44,00	46,00	55,00	

hmay=50

kcell/seq	S7	S9	S12
1,00	14,28	10,12	10,80
1,25	30,25	13,33	16,07
1,50	20,67	20,17	27,12
1,75	31,12	32,50	44,83
2,00	51,78	49,38	61,28

hmax=75

### Main nonlinear minimization scheme

```
// MAIN SCHEME:
Main(Sh, f, tolAdapt, errm)
  Initialize (Th, Qh; Sh, f); // Initialization of Th and Qh.
  NbOfAdapt = length(tolAdapt); // Total nb of adaptations.
  int k=0;
                          // Adaptation index is initialized.
  Qh= Calculate_Nematic_Structure(Th, tolAdapt_k);
  while (++k < NbOfAdapt) {
     Th= Adapt_Mesh(Th, Qh, errm_k);
     Qh= Calculate_Nematic_Structure(Th, tolAdapt_k);
  return Th, Qh;
```

# Mesh adaptivity procedure

```
// MESH ADAPTATION:
Adapt_Mesh(Th, Qh; hmax, errm_k) // Other possible parameters:
                                  // hmin, hgrad (here fixed).
  mesh3 Thx= Th; // Declares and initializes new mesh variable.
  scFields= {Qh, S, DF}; // Scalar fields for metric calculus.
  for (j=1; j<=NAdaptIter; ++j) {</pre>
     fespace Vhx(Thx, P13d); // Declares new FE space.
     Vhx M= mshmet(Thx, scFields, hmin, hmax, errm_k);//Metric.
     Thx= mmg3d5ljll(Thx, M, hmin, hmax, hgrad); // Remeshing.
     if (meshes close enough) break; // Loop-exit condition.
  return Th=Thx, Qh;
```