Mesh refinement techniques applied to neutron balance equations,

and then some ...

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Outline

- **Background info**
  - Short bio
  - Research thrust areas
    - Computational-based science
    - Nuclear System Analysis and Design
- **Mesh Refinement Techniques**
  - Why do mesh adaptation?
  - How to do it?
  - Application to multigroup diffusion and SPN eqs
  - Sn Transport case: work in progress
- **Neutron Transport Inverse Problems**

Background info

- 1996 : **Diplôme d'ingénieur**, Engineering school of Physics, Grenoble, France
- 1996 : M.S., Nuclear Engineering, Texas A&M University, **Research Assistant**
- 1997 : **Military Service (engineer),** Commissariat à l'énergie Atomique (CEA, Bruyères-le-Châtel, France)
- 1998/2001 : Ph.D., Nuclear Engineering, National Polytechnic Institute of Grenoble, France (**Research Fellow** at the CEA, Saclay, France)
- 2001 : **Visiting Assistant Professor**, School of Nuclear Engineering, Purdue University
- 2002/2004 : **R&D Engineer**, Commissariat à l'énergie Atomique (CEA, Saclay), Department of Applied Mathematics and Reactor Studies.
- 2004/pres. : **Assistant Professor**, Nuclear Engineering, Texas A&M University

Research thrust areas:

- **Computational-based science**
  - **Pushing the limits in simulation-based applications for nuclear engineering in**
    - **Reactor Analysis / Shielding Methodology,**
    - **Neutron Transport Inverse Problems (Smuggled Nuclear Material Detection).**

- **Reactor Analysis and Design**
  - **Improving the cost savings and safety margins of nuclear fuel assemblies and cores**
    - **Optimization for Minor Actinides and Transuranics management,**
    - **Optimization for higher burn-up capabilities.**

Projects, Sponsors, and Supported Students

Topic	Grant / contract	Collaborators
Mesh Adaptation for Neutron Transport Applications	DOE (JFA)	ORNL
Multi-physic Coupling and Fast Reactor Safety Analysis	DOE (NERI) INL	INL ANL CEA
Cargo Container Detection (Neutron Transport Inverse Problem)	DOE (NEER)	TAMU (Dr. Bangerth, Math; Dr. Charlton, Nuen)

Note: Photographs have been removed

Yaqi

Alissa

Adam

Vijay

Mark

Projects, Sponsors, and Supported Students

Topic	Grant / contract	Collaborators
Fuel Assembly Design for the Next Generation of LWRs	DOE (NERI)	TAMU (Dr. Vierow, Nuen)
Fuel Assembly Optimization	Duke Energy	
Fast Reactor Safeguards	DOE-NA24	TAMU (Drs. Charlton & Nelson, Nuen)

Note: Photographs have been removed

Bryan

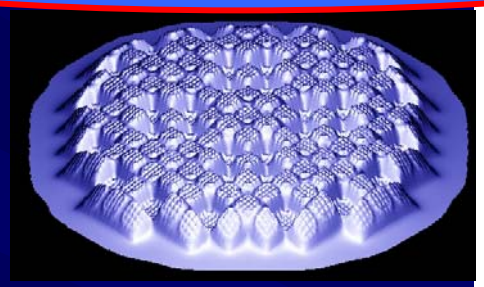
Adam

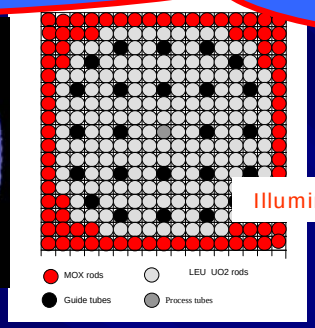
Tim

Rich

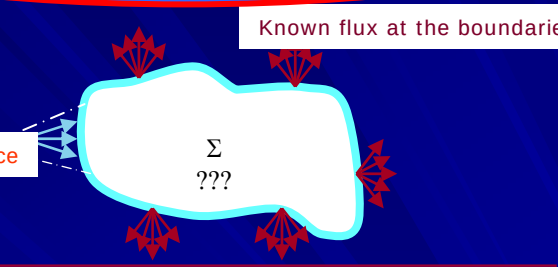
Brief “picturesque” research interests

Reactor core and assembly designs



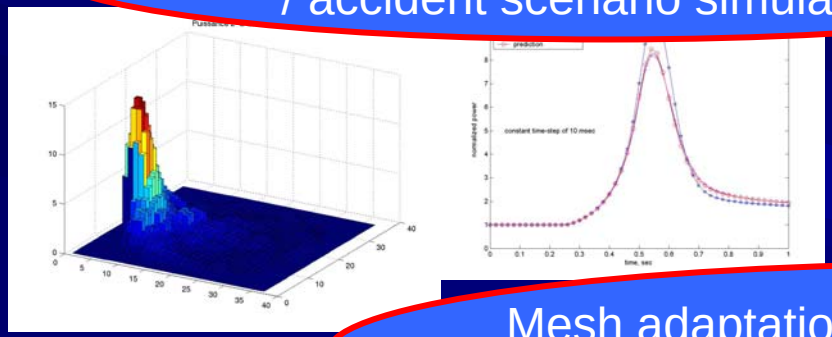


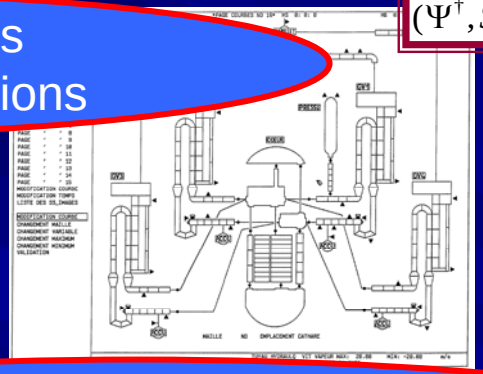
Smuggled Material Detection Methodology



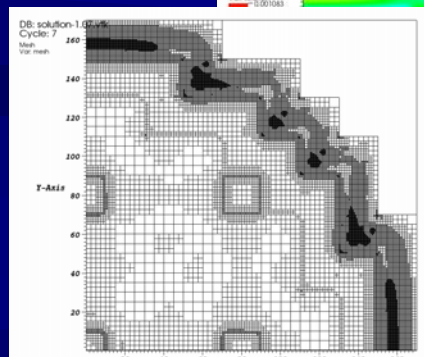
$$(\Psi^{\dagger}, S) + < \Psi^{\dagger}, \Psi_{in} >_{-} = (S^{\dagger}, \Psi) + < \Psi^{\dagger}_{out}, \Psi >_{+}$$

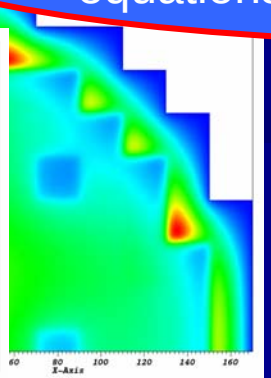
High fidelity multi-physics
/ accident scenario simulations

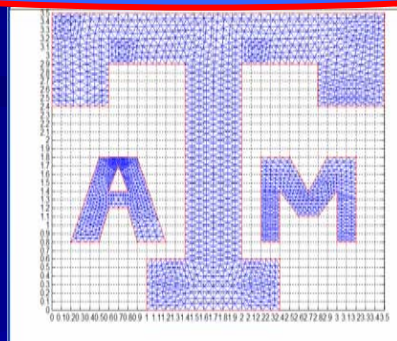


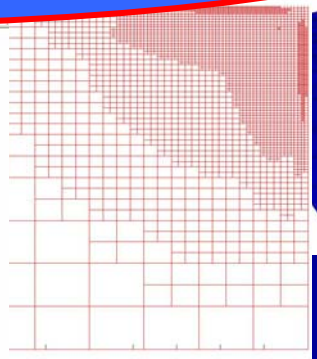


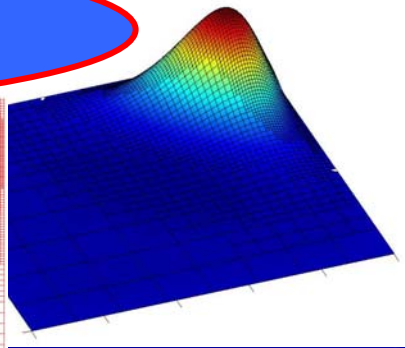
Mesh adaptation for solving neutron balance equations accurately on complex geometries











Foreword : Needs related to High-fidelity simulations

- Numerical error is **intrinsic** to any computer simulation of physical phenomena.

- Requirements for HiFi:
  - To **automatically** monitor the numerical error
  - To obtain **guaranteed solutions (**solutions converged to a desired, i.e., user prescribed, tolerance)
  - To obtain guaranteed **quantities of interest** (i.e., functionals of the solution)

- Tools:
  - **Error estimates**
  - **Automated mesh refinement strategies**
  - **Dual (adjoint) problems**

Mesh adaptation: what is that?

- Engineering problems are complex → no analytical solutions are available for real-life problems → **numerical** methods → need to mesh the domain / need to pick a method to discretize the PDEs
- A **numerical** solution can be improved by
  - Either refining the grid (i.e., put more meshes)
  - Or increasing the solution space (i.e., augmenting the polynomial order)
  - **Or both !**
- The **refinement** can either be:
  - **Uniform** : All mesh cells are divided, poly. order is uniformly increased.
  - **Adaptive** : Only **selected** cells will be divided/will have their poly. order increased.
- Classical approaches such as uniform mesh refinement will **not** tell you about the achieved accuracy (unless you run a finer computation!!!). Usually, uniform refinement is:
  - CPU expensive,
  - Not automated,
  - Not the best use of an engineer's time !!!

Mesh adaptation: what is that?

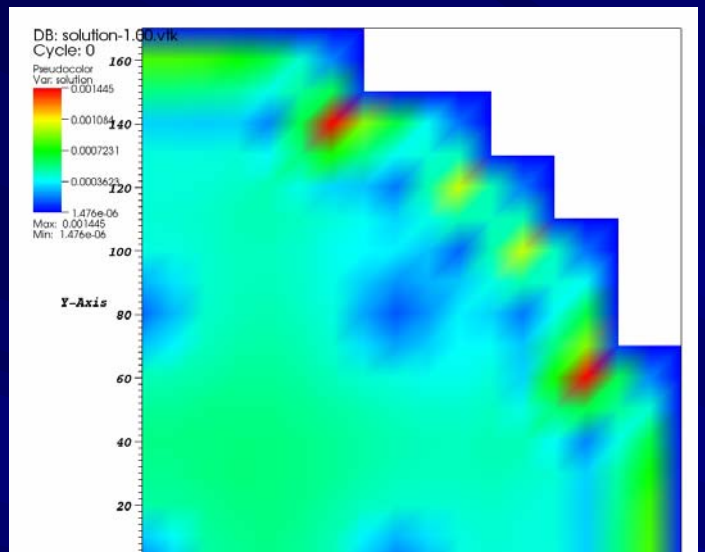
- How to **select meshes for refinement**???
  - The effort put into the numerical solution **must be driven by the accuracy** required (user's choice)

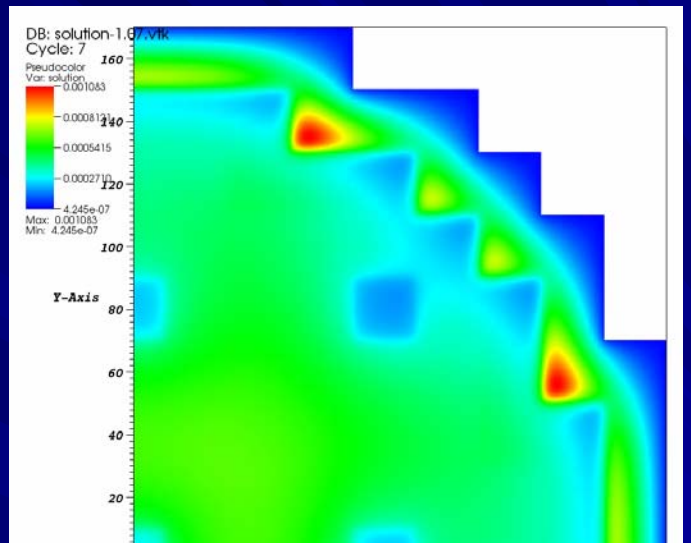
- Additionally, do you need accuracy everywhere in the mesh ???
  - **No**, obtaining a highly accurate solution everywhere may not be desired from an engineering Point of View:
    - Reaction rate in a sub domain (e.g, power in a pin, or detector reaction rate)
    - Or the flux (or the current) at a point (e.g., after a thick shield).
  - We develop **goal-oriented** approaches for **specific quantities of interest**.

- Our work: to use/devise algorithms that
  - automatically (user-independent)
  - adapt the mesh (sensible usage of the resources)
  - to a user-prescribed tolerance (guaranteed accuracy)
  - for a specific quantity of interest (goal-driven)

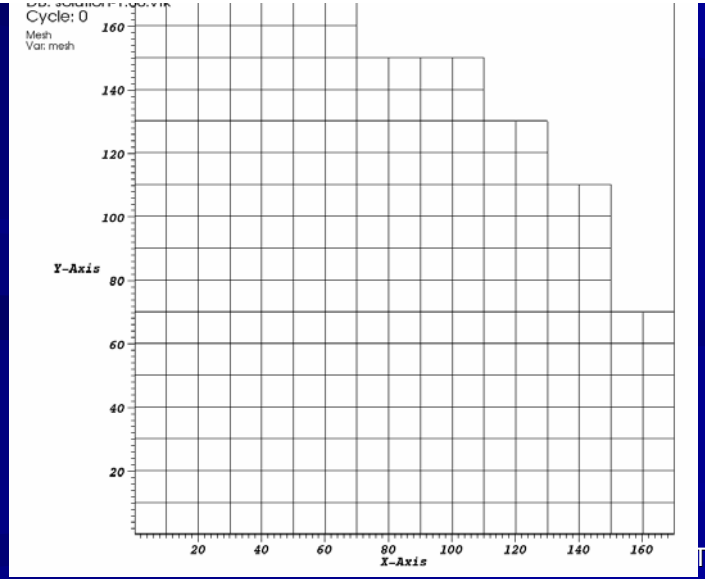
A picture is better than a thousand words …

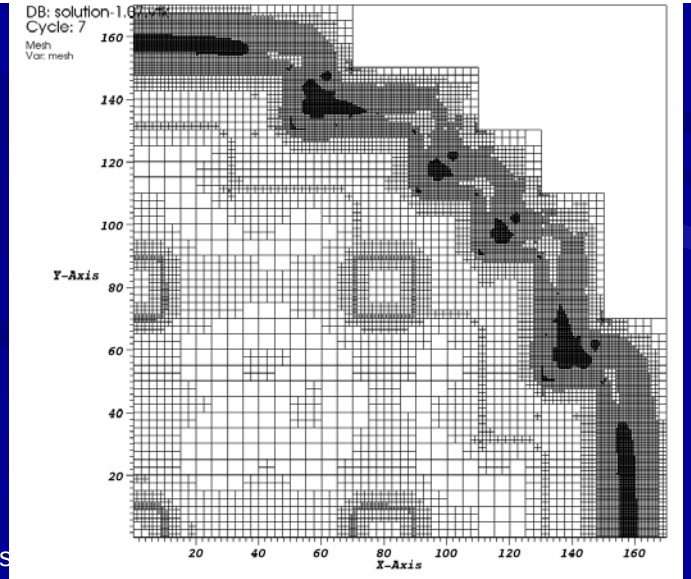
- IAEA 2D benchmark solved using 2-g diffusion:





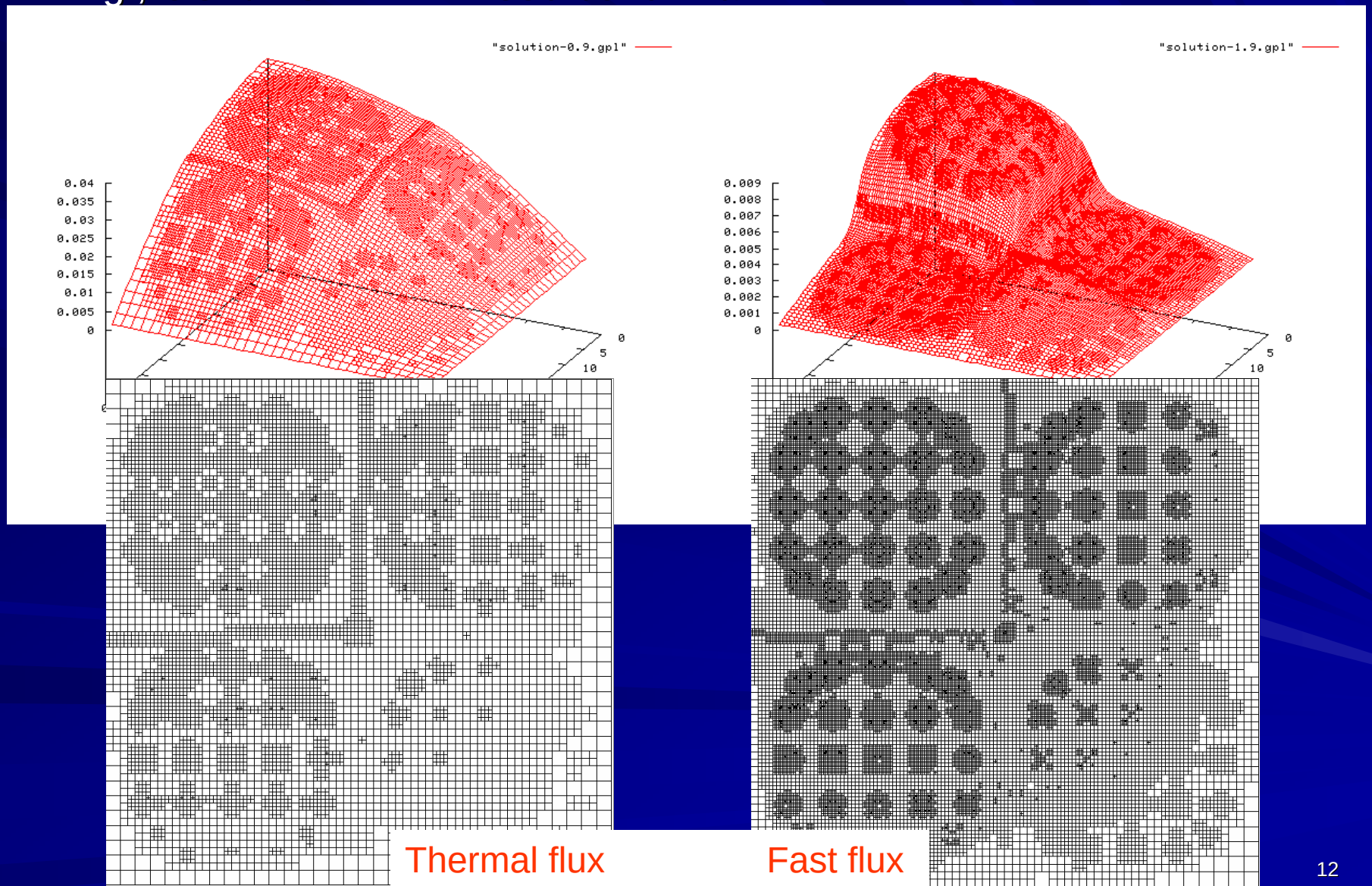
Thermal flux on the initial mesh (left) and at mesh iteration #8 (right)





A picture is better than a thousand words …

- Fast flux solution is typically smoother than the thermal flux solution.
- E.g., UOX/MOX NEA-L-336 benchmark:



FEM 101

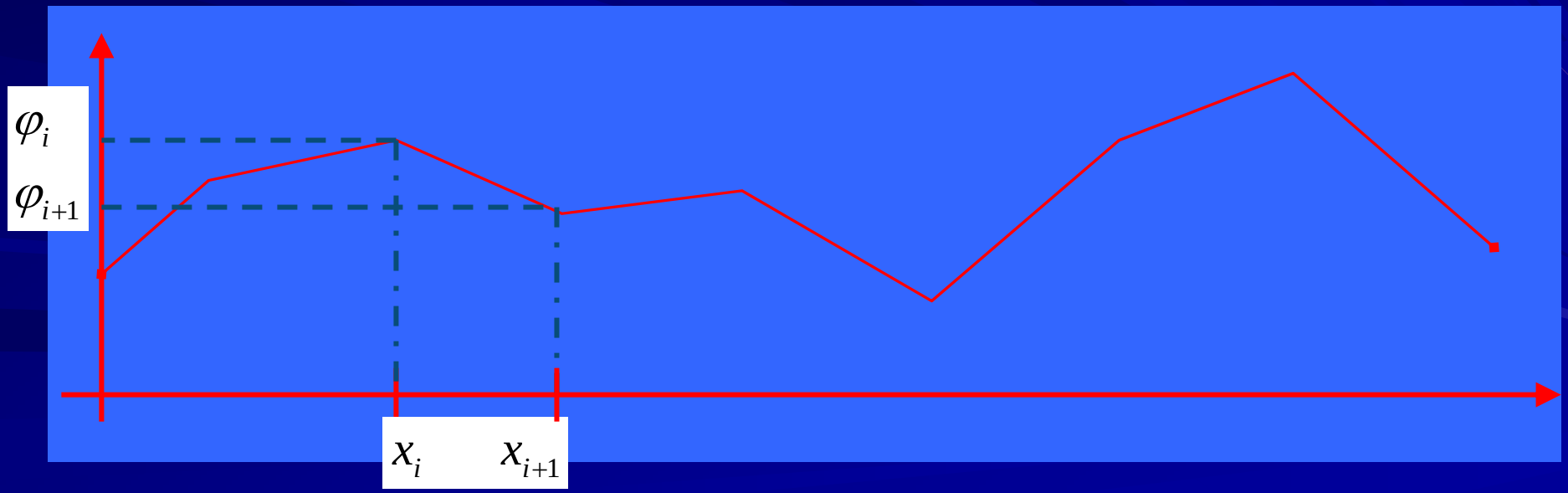
- Simple diffusion eq.:

$$-\frac{d}{dx}D\frac{d\phi}{dx}+\Sigma_a\phi=S \quad \text{on } 0\le x\le L \quad + \text{B.C.}$$

- Get a mesh → subdivide segment [0,L] into *N* smaller segments [x_i,x_{i+1}]

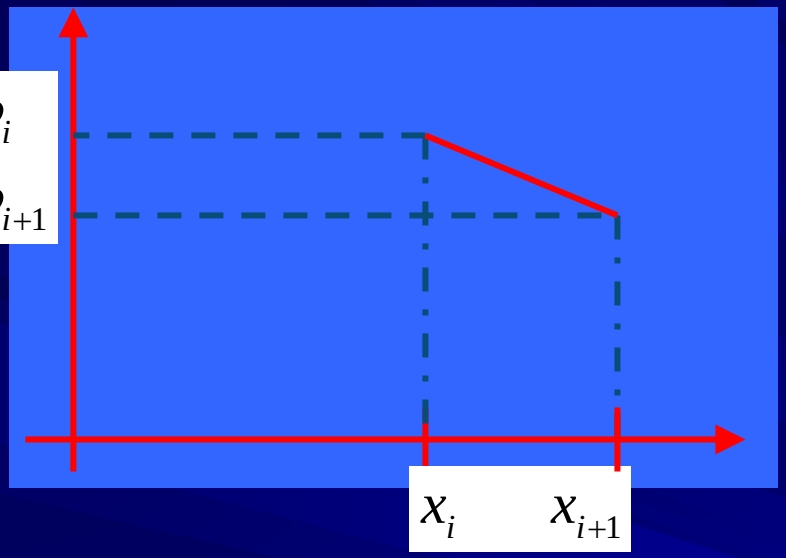
- Seek the flux as a linear continuous function

$$\phi(x)=\sum_{i=0}^{i=N}\varphi_i B_i(x) \qquad \varphi_i \text{ are the } N+1 \text{ unknown coefficients}$$

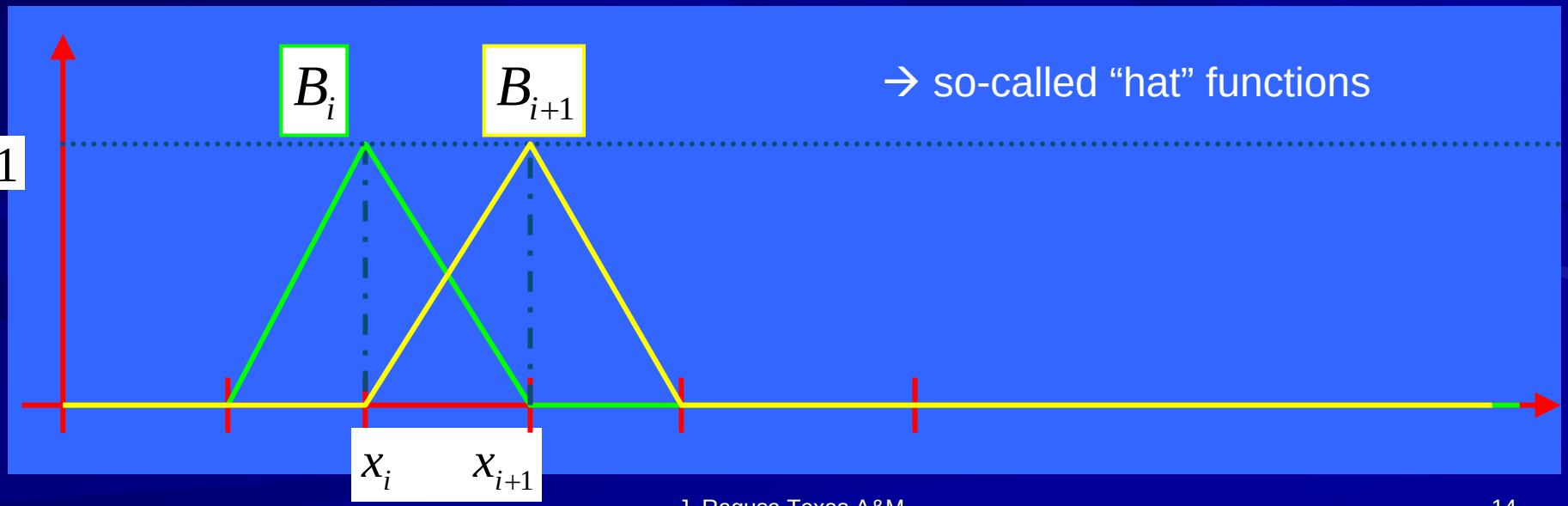


FEM 101

- A little more on the basis functions



$$\varphi_i \underbrace{\frac{x_i - x}{x_{i+1} - x_i}}_{B_i\big|_{\text{element i}}} + \varphi_i \underbrace{\frac{x - x_{i+1}}{x_{i+1} - x_i}}_{B_{i+1}\big|_{\text{element i}}}$$



→ so-called “hat” functions

FEM 101

- 1 eq. but so many unknowns !

$$-\frac{d}{dx}D\frac{d\left[\sum_{i=0}^{i=N}\varphi_i B_i(x)\right]}{dx}+\Sigma_a\left[\sum_{i=0}^{i=N}\varphi_i B_i(x)\right]=S$$

- Idea: pre-multiply this equation by any B_j ($0\le j\le N$) and integrate over the entire domain [0,L] → obtain enough equations to solve for the unknowns

$$-\int_0^L\frac{d}{dx}D\frac{d\left[\sum_{i=0}^{i=N}\varphi_i B_i(x)\right]}{dx}B_j(x)dx+\int_0^L\Sigma_a\left[\sum_{i=0}^{i=N}\varphi_i B_i(x)\right]B_j(x)\mathrm{dx}=\int_0^L S(x)B_j(x)dx$$

- Perform integration by parts (→reduces requirements on the *B*'s)

$$\sum_{i=0}^{N}\varphi_i\left\{\int_0^L\frac{dB_j}{dx}D\frac{dB_i}{dx}dx\right\}+\sum_{i=0}^{N}\varphi_i\left\{\int_0^L\Sigma_a B_i(x)B_j(x)dx\right\}=\int_0^L S(x)B_j(x)dx$$

(+BC treatment) for any $0\le j\le N$

PDE's 101

- The multigroup diffusion equations are
  - Elliptic
  - Positive Definite (but not SPD)

- As such, the '*natural*' norm to analyze/quantify the error is the H-1 norm

$$\boxed{\|\phi\|^2_{H^1(\Omega)} = \left[\int_\Omega \nabla\phi\cdot\nabla\phi + \phi^2\right] = |\phi|^2_{H^1(\Omega)} + \|\phi\|^2_{L^2(\Omega)}}$$

- A technical nicety (Poincare's inequality). It is sufficient to use the semi-H-1 norm

$$|\phi|^2_{H^1(\Omega)} = \int_\Omega \nabla\phi\cdot\nabla\phi$$

→ fewer computations

PDE's 102

- The variational boundary value formulation of the multigroup equations is:

$$\boxed{b(\phi,\varphi) = f(\varphi), \quad \phi \in \phi_D + \mathrm{X} \subset H^1(\Omega), \ \forall \varphi \in \mathrm{X}}$$

where the terms of the bilinear and linear forms are:

$$b(\phi,\varphi) = \sum_{g=1}^{G}\left[\int_\Omega \left\{D^g \nabla\varphi^g \cdot \nabla\phi^g + \Sigma_r^g \varphi^g \phi^g\right\} dr + \tfrac{1}{2}\int_{\partial\Omega_C} \varphi^g(r_b)\phi^g(r_b)dr_b\right]$$

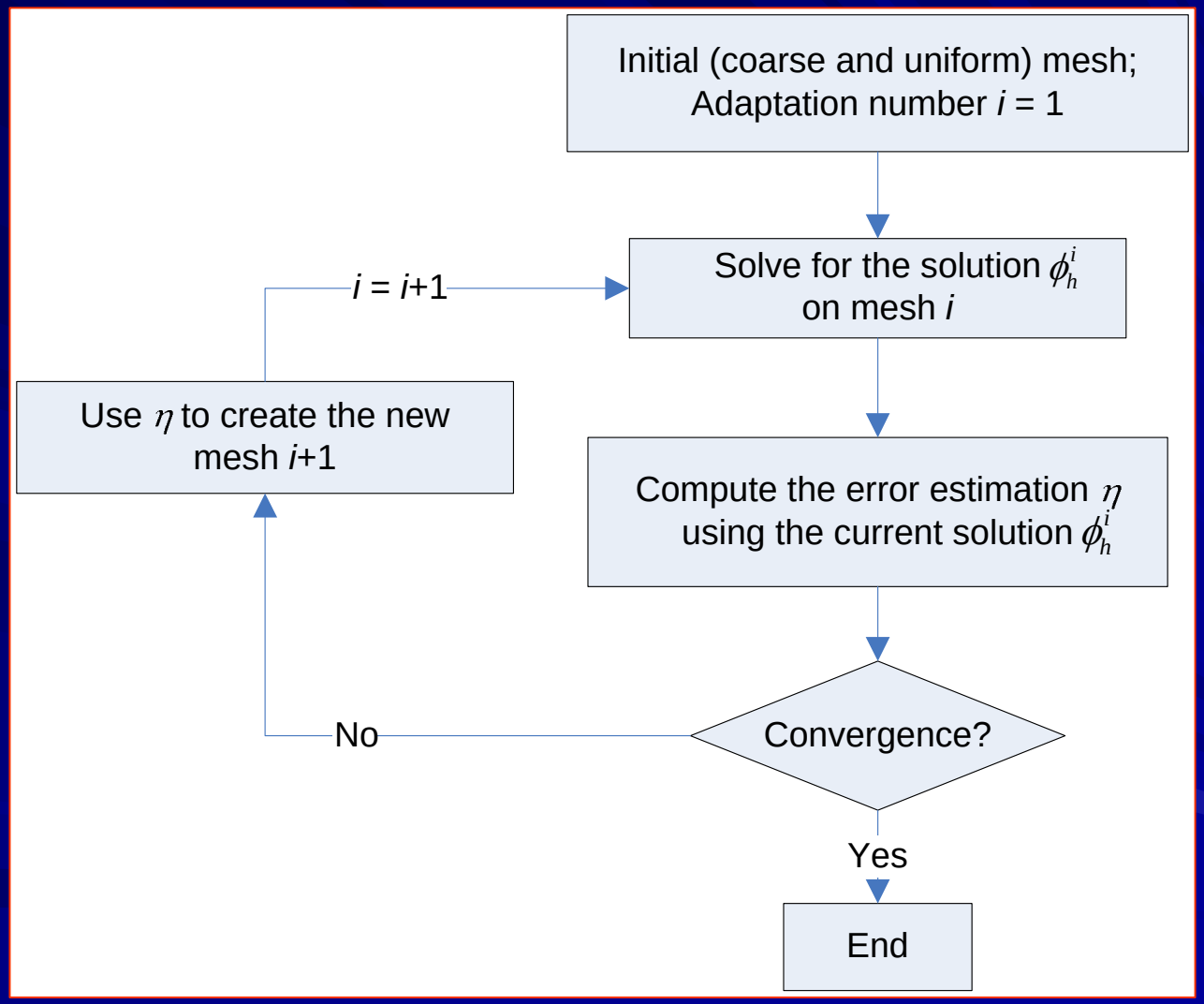
$$-\sum_{g=1}^{G}\sum_{g'\neq g}\int_\Omega \Sigma_s^{g\to g'}\varphi^{g'}\phi^g dr - \sum_{g=1}^{G}\sum_{g'}\int_\Omega \chi^g{}' \nu\Sigma_f^g \varphi^{g'}\phi^g dr \ .$$

$$f(\varphi) = \sum_{g=1}^{G}\left\{\int_\Omega S_{ext}^g(r)\varphi^g(r)dr + \int_{\partial\Omega_N} J_N^g(r_b)\varphi^g(r_b)dr_b + 2\int_{\partial\Omega_C} J_C^g(r_b)\varphi^g(r_b)dr_b\right\}.$$

- Also, note that the bilinear inner product is a norm equivalent to the H-1 norm (and to the semi-H-1 norm, cf. Poincare's inequality)

$$b(\phi,\phi) = \left[\int_\Omega D\nabla\phi\cdot\nabla\phi + \Sigma\phi^2\right] \sim \text{equivalent to } \|\phi\|^2_{H^1(\Omega)}$$

Mesh adaptation: principles



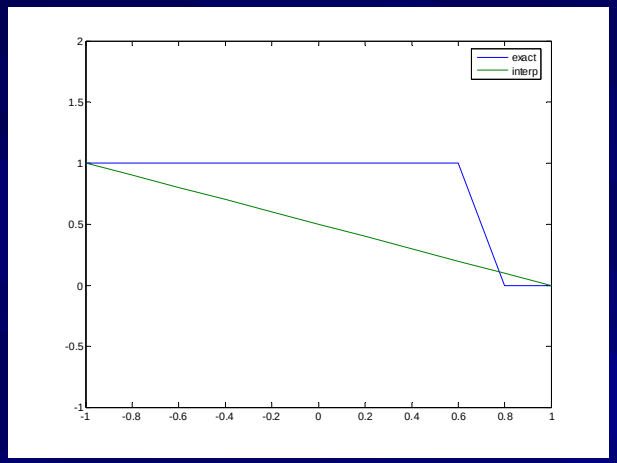
Adaptive Mesh Refinement: refinement options

- *h*-refinement:
  - Selective subdivision of the mesh, the polynomial order is kept fixed
  - Good for singularities in the solution (boundary singularities, data singularities)
  - Not optimal for regions where the solution is smooth (e.g., if the true solution is quadratic, a linear approximation would still require some mesh subdivision to be performed)
- *p*-refinement:
  - The initial mesh is kept unchanged, selective increase in the polynomial order
  - Good for computing a smooth solution with large mesh cells
  - Not optimal for singularities
- *hp*-refinement:
  - Combines *h*-refinement and *p*-refinement

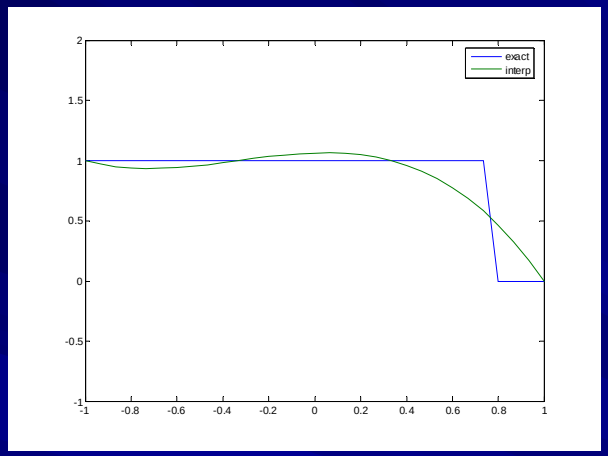
h versus p: (1/2)

- Suppose your solution is not smooth, increasing the polynomial order will get you nowhere.

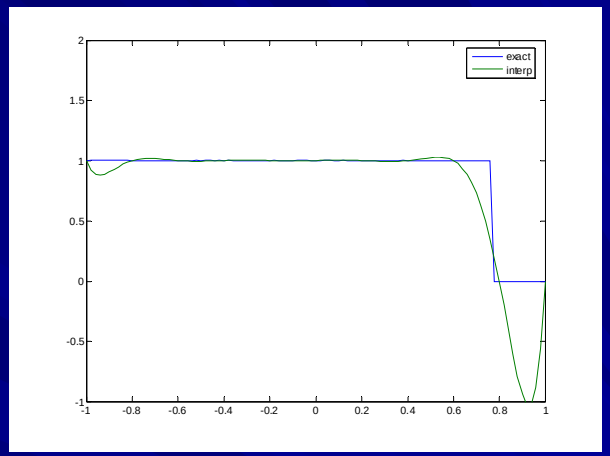
p = 1



p = 3



p = 10



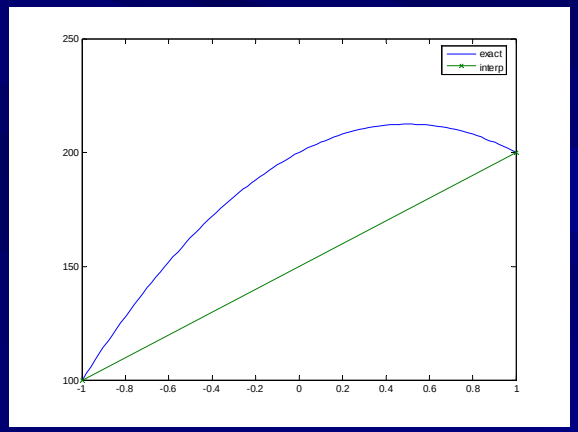
- You'd be better off cutting the interval into 3 subintervals and use linear functions in each new interval.

- In this example, the number of unknowns is:
  - One interval, p=10 → 11 unknowns
  - 3 intervals, p=1, → 4 unknowns !!!!

h versus p: (2/2)

- Suppose your solution is smooth (say quadratic, i.e., p=2), then the **exact** solution is given by an approximation using only one interval and a polynomial order of 2 !!!
- On the other hand, using linear functions but Increasing the number of intervals will get you somewhere (but slowly).

= 1



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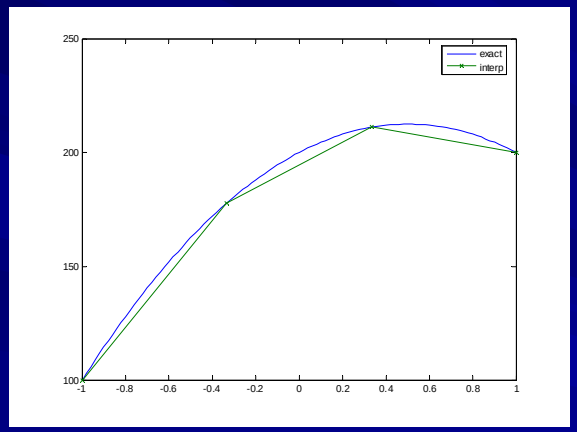
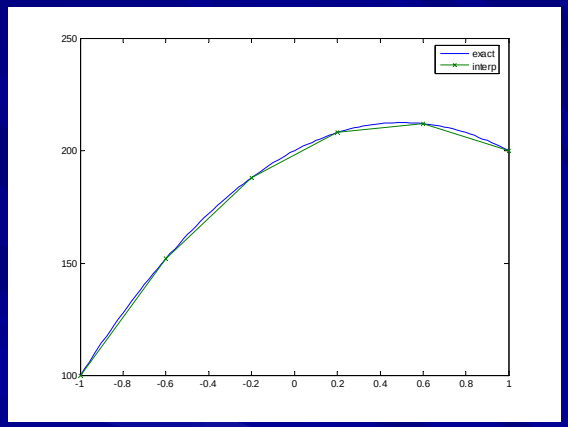


= 5



- You'd be better off using a higher polynomial order approximation.
- In this example, the number of unknowns is:
  - One interval, p=2 → 3 unknowns
  - 5 intervals, p=1, → 6 unknowns !!!!

hp-Adaptive Mesh Refinement: convergence rates

Refinement strategy	Error $\left\|e_{hp}\right\|_{H^1(\Omega)}$ proportional to	Log of the error as a function of the number of unknowns *N*
Uniform *h*-refinement	$h^{\min(p,r)}$	$-\min(p,r)\times\log(N)$
Adaptive *h*-refinement	h^{p}	$-p\times\log(N)$
Uniform and adaptive *p*-refinements	p^{-r}	$-r\times\log(N)$
Adaptive *hp*-refinement	$e^{-\alpha N^{\theta}},\ \ \alpha>0,\ \theta=\frac{1}{2d-1}$ where d is the problem's dimension	$-\alpha\times N^{\frac{1}{2d-1}}$

- ❑ *hp*-refinement provides exponential convergence (seminal work by Babuska et al.)
- ❑ *h*-refinement only possesses algebraic convergence rates

Multigroup issues in mesh adaptation

- The smoothness of the flux in a given energy group depends on the smoothness of the data (XS and rhs).
  - Fast flux: usually much smooth than thermal flux
  - → Do not use the same mesh for each group !!!

- Yeah, but what about the coupling in group g due :
  - to scattering from other groups g' to group g
  - to fission from other groups g' to group g

$$-\vec{\nabla}\cdot(D_g(x)\vec{\nabla}\phi_g(x))+\Sigma_{r,g}(x)\phi_g(x)=\frac{1}{k_{eff}}\chi_g\sum_{g'=1}^{G}\nu\Sigma_{f,g'}(x)\phi_{g'}(x)+\sum_{g'\neq g}\Sigma_{s,g'\to g}(x)\phi_{g'}(x)$$

$$g=1,2,\cdots,G$$

Multigroup issues in mesh adaptation

- → adaptive integration:

$$\int_{K^g} B^{p^g}_{K^g} B^{p^{g'}}_{L^{g'}}\Big|_{K^g} = \sum_n \int_{K^g_n} B^{p^g}_{K^g}\Big|_{K^g_n} B^{p^{g'}}_{L^{g'}}\Big|_{K^g_n}$$

$$= \sum_n \sum_i w_i B^{p^g}_{K^g}\Big|_{K^g_n}(x_i) B^{p^{g'}}_{L^{g'}}\Big|_{K^g_n}(x_i)$$

Instead of integrating over the whole element K^g , we split it into subintervals and integrate over each subinterval separately and then add the corresponding contributions.

  – The subintervals are determined adaptively as needed.

- → analysis of the refinement depth:

For a given cell,

  – look-up the difference in refinement levels between group g and other groups g',
  – then project/restrict the basis functions of groups g' accordingly,
  – and finally use a numerical quadrature to perform the integral.

Mesh adaptation applications: MG diffusion / SPN

- Multigroup Diffusion and Simplified PN Transport (SPN) equations
- Ongoing work : Multigroup SN Transport equations

- Application examples:

A. **Standard** adaptivity with 3 different error estimates:
   1. Projection-based interpolation (hp-adaptivity in 1D, diffusion)
   2. Hessian-based (h-adaptivity, multi-D , diffusion)
   3. Error jump-based (h-adaptivity, multi-D , diffusion **and** SPN)

B. **Goal oriented** adaptivity:
   1. Projection-based interpolation (hp-adaptivity in 1D, diffusion)

hp-Adaptive Mesh Refinement: error estimates

- The key is to use a powerful lemma (Céa's lemma), which states that the **approximation error is bounded by the interpolation error** in the H-1 norm.

$$\left\| e_{hp} \right\| = \left\| \phi - \phi_{hp} \right\| \le C \left\| \phi - \Pi_{hp} \phi \right\|$$

- The role of the exact solution ϕ will be played by a *reference* numerical solution:

$$\left\| e_{hp} \right\| = \left\| \phi - \phi_{hp} \right\| \le C \left\| \phi_{hp-fine} - \Pi_{hp-coarse} \phi_{hp-fine} \right\|$$

- Let us call the **current** *hp*-mesh the "*hp-fine*" mesh and let us denote it by $h/2,p+1$

$$\phi \approx \phi_{hp-fine} = \phi_{h/2,p+1}$$

- The "*hp-coarse*" mesh is simply a coarsening of the "*hp-fine*" mesh and let us denote it by h,p

- The local error in a given cell *K* is, therefore, given by

$$\eta_K = \left\| \phi_{h/2,p+1} - \Pi_{hp} \phi_{h/2,p+1} \right\|_{H^1,K}$$

hp-Adaptive Mesh Refinement: error estimates

- The adaptation process has **converged** when the relative error is within a user-prescribed tolerance

$$\sum_K \frac{\eta_K}{\left\|\phi_{h/2,p+1}\right\|_{H^1,K}} = \sum_K \frac{\left\|\phi_{h/2,p+1} - \Pi_{hp}\phi_{h/2,p+1}\right\|_{H^1,K}}{\left\|\phi_{h/2,p+1}\right\|_{H^1,K}} < \varepsilon_{USER}$$

- Otherwise, we will **mark** for refinement all elements such that:

$$\eta_K \geq \frac{1}{3}\max_{K'} \eta_{K'}$$

(bulk error chasing)

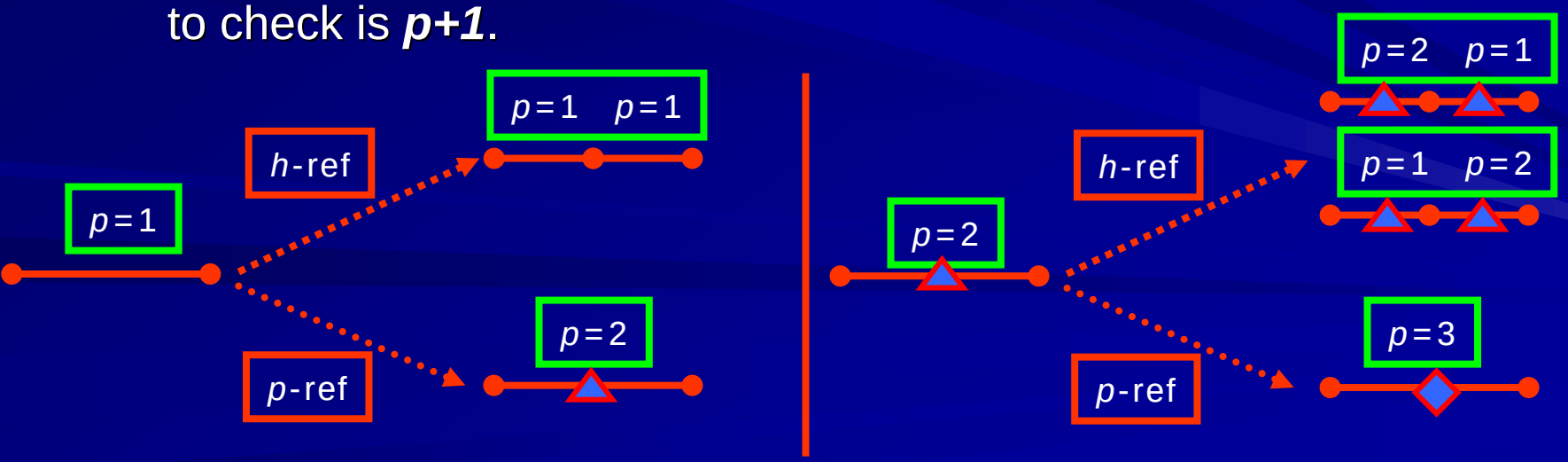
- Again, **only** $\phi_{h/2,p+1}$ needs to be solved for.
- All other computations are simply projections and norms (i.e., integrals) performed cell by cell !

hp-Adaptive Mesh Refinement: competitive refinement

- At this point, we are ready to competitively choose the best refinement mode **for each element** [i.e., *h*- or *p*-refinement →***hp*-refinement**].
  - If ***p***-refinement is chosen, we keep the current mesh but increase the polynomial order by 1: $h_K^{new} = h_K^{old} \quad \text{and} \quad p_K^{new} = p_K^{old} + 1$
  - If ***h***-refinement is chosen, we keep the old poly. order but subdivide the mesh:

$$h_{K,left}^{new} = h_{K,right}^{new} = \frac{h_K^{old}}{2}, \quad \text{and} \quad p_{K,left}^{new} + p_{K,right}^{new} = p_K^{old} + 1$$

  - For an element of initial polynomial degree *p*, the number of cases to check is ***p+1***.



hp-Adaptive Mesh Refinement: competitive refinement

- Our goal is to go for the **maximum error reduction** with the minimum increase in the number of unknowns (degrees of freedom or DOF in the FE jargon).

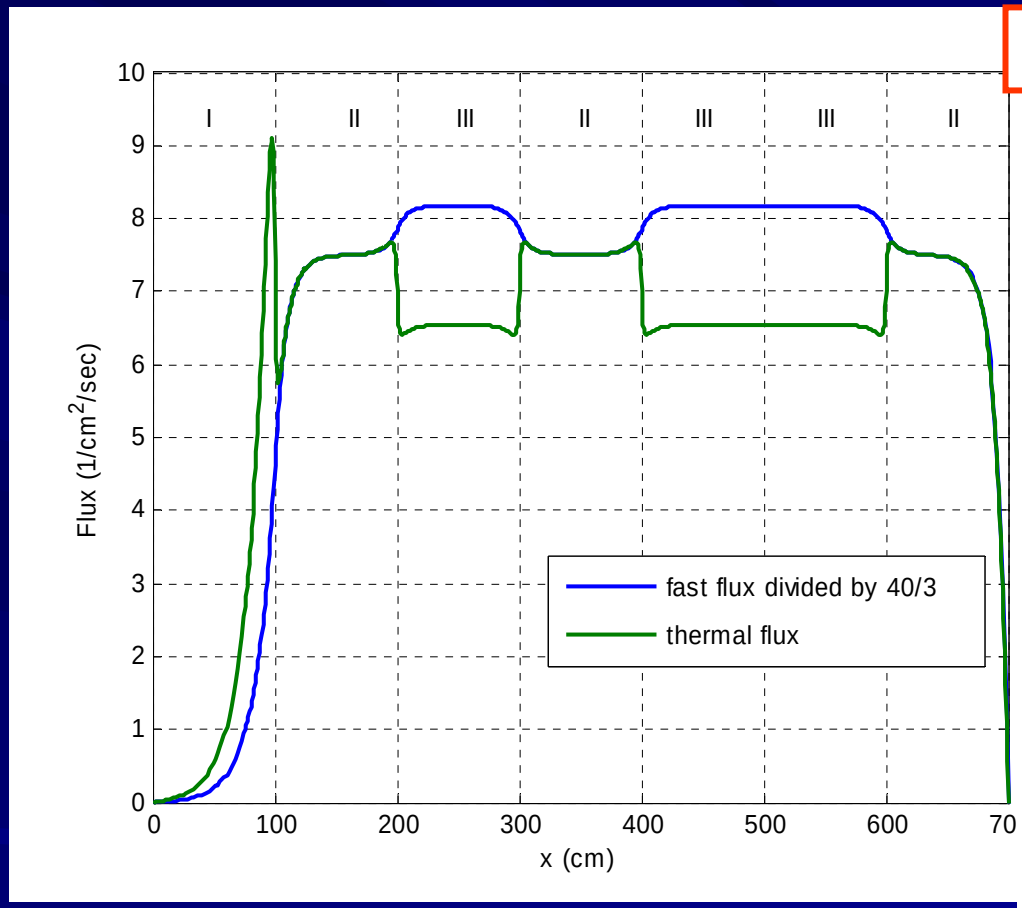
- The optimal local refinement choice driven by the rate of decrease in the error:

$$\frac{\left\| \phi_{h/2,p+1} - \Pi_{h^{old} p^{old}} \phi_{h/2,p+1} \right\|_{H^1,K} - \left\| \phi_{h/2,p+1} - \Pi_{h^{new} p^{new}} \phi_{h/2,p+1} \right\|_{H^1(K)}}{1}$$

Local quantity !!!

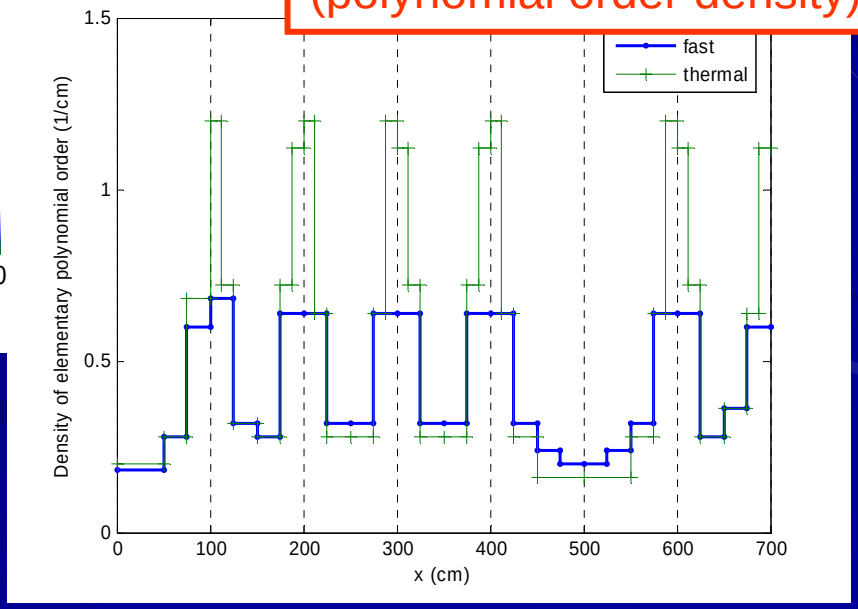
hp-Adaptive Mesh Refinement: some results

- Two-group 7-region eigenproblem



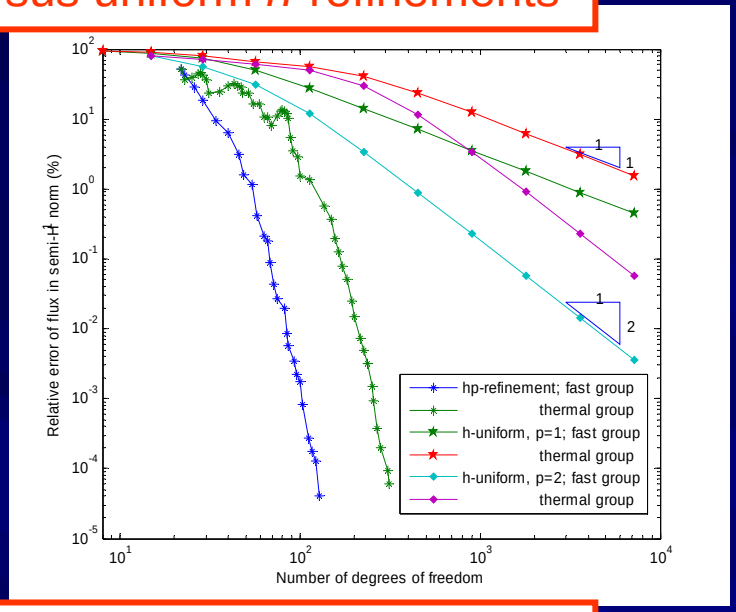
hp- solution

hp- mesh
(polynomial order density)

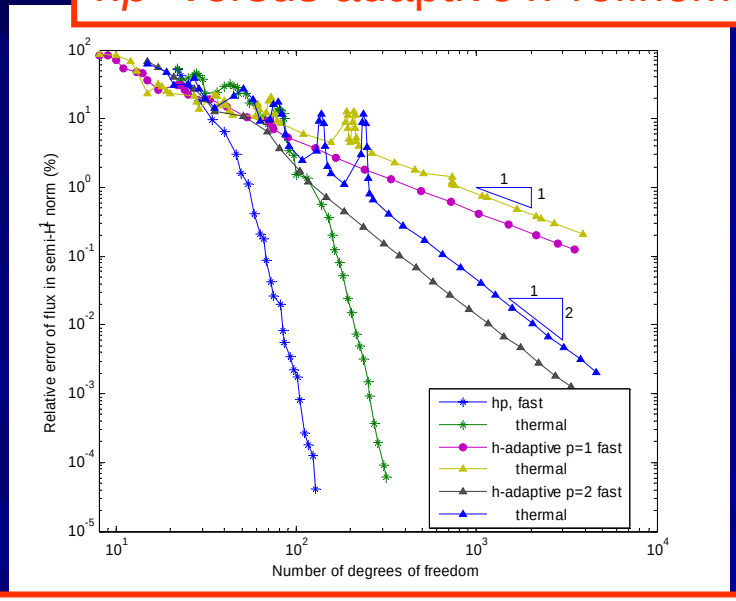


hp-Adaptive Mesh Refinement: Log(err) vs. unknowns

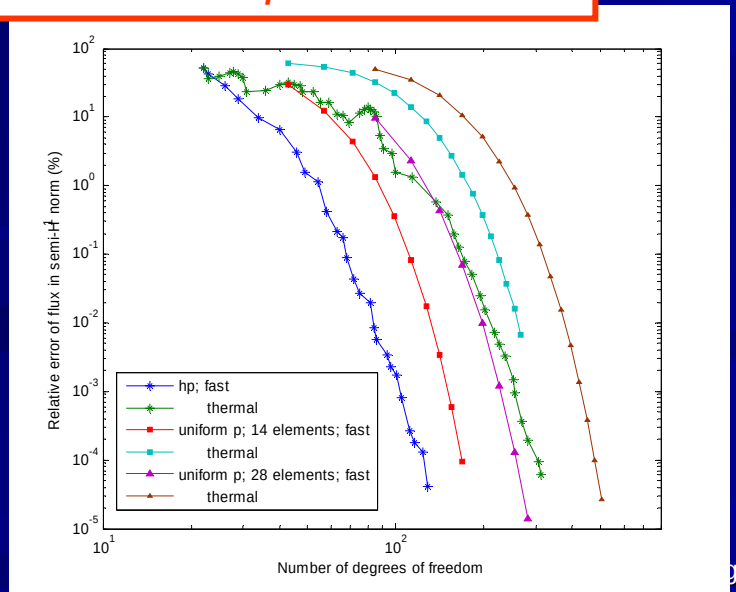
hp- versus uniform *h*-refinements



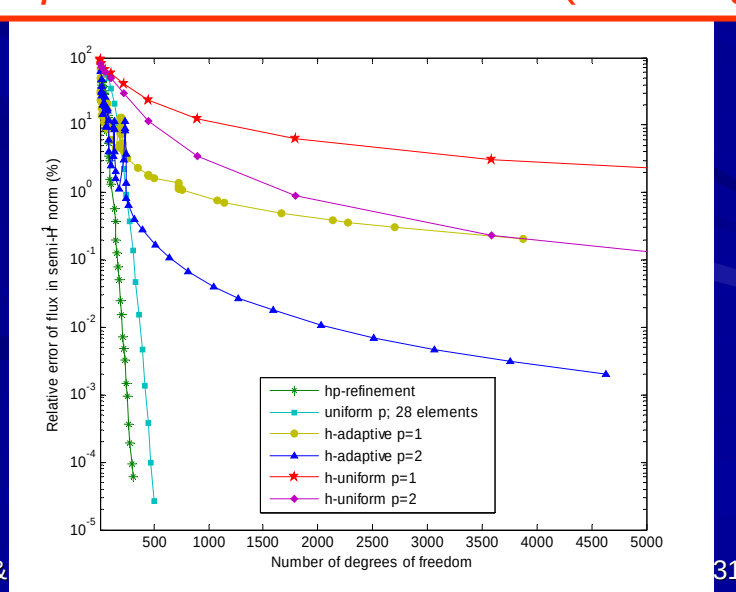
hp- versus adaptive *h*-refinements



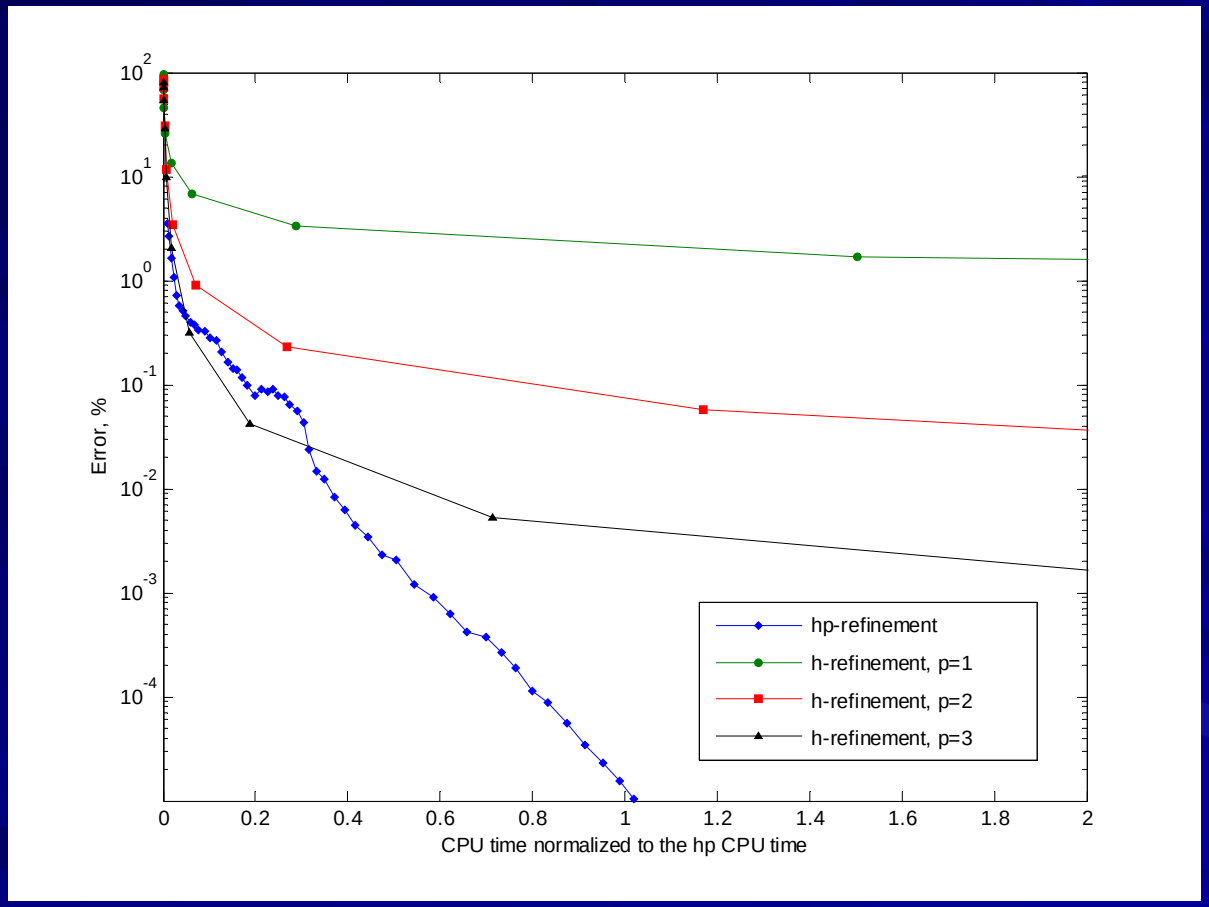
hp- versus uniform *p*-refinements



hp- versus *h*-refinements (semi log plot)



hp-Adaptive Mesh Refinement: CPU cost



Mesh adaptation applications: MG diffusion / SPN

- Multigroup Diffusion and Simplified PN Transport (SPN) equations
- Ongoing work : Multigroup SN Transport equations

- Application examples:

A. **Standard** adaptivity with 3 different error estimates:
   1. Projection-based interpolation (hp-adaptivity in 1D, diffusion)
   2. Hessian-based (h-adaptivity, multi-D , diffusion)
   3. Error jump-based (h-adaptivity, multi-D , diffusion **and** SPN)

B. **Goal oriented** adaptivity:
   1. Projection-based interpolation (hp-adaptivity in 1D, diffusion)

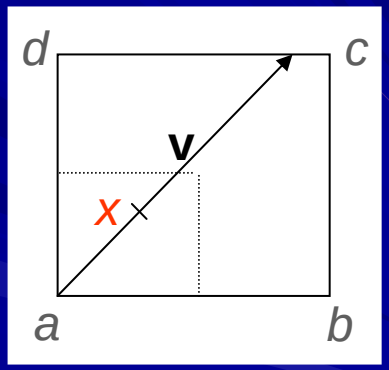
Hessian-based h-adaptivity

- Starting from Cea's lemma, (approximation error is controlled by interpolation error)

$$\|e_h\| = \|\phi - \phi_h\| \le C\|\phi - \Pi_h \phi\|$$

- But let's do a Taylor series expansion of the interpolation error. Let's choose a square element and start the TSE from one of its corner.

$$(u - \Pi_h u)(\boldsymbol{a}) = (u - \Pi_h u)(\boldsymbol{x}) + \left\langle \boldsymbol{x} - \boldsymbol{a}, \vec{\nabla}(u - \Pi_h u)(\boldsymbol{x}) \right\rangle + \int_0^1 dt \left\langle \boldsymbol{x} - \boldsymbol{a}, H_u\left(\boldsymbol{x}(1-t) + t\boldsymbol{a}\right)(\boldsymbol{x} - \boldsymbol{a}) \right\rangle$$



- No interpolation error at **a**
- Interpolation error is maximum (i.e., its gradient =0) at

some point **x** for element *K*:

$$\varepsilon_h^K = \max_{\boldsymbol{x} \in K} \left|(u - \Pi_h u)(\boldsymbol{x})\right| = \max_{\boldsymbol{x} \in K} \left| \int_0^1 dt \left\langle \boldsymbol{x} - \boldsymbol{a}, H_u\left(\boldsymbol{x}(1-t) + t\boldsymbol{a}\right)(\boldsymbol{x} - \boldsymbol{a}) \right\rangle \right|$$

Hessian-based h-adaptivity

- Use vector **v** and decompose on the element's edges

$$\left\| u - \Pi_h u \right\|_{\infty,K} = \varepsilon_h^K \le c \max_{\mathbf{v}\in \mathrm{K}} \max_{\boldsymbol{x}\in K} \left\langle \mathbf{v}, \left| H_u(\boldsymbol{x}) \right| \mathbf{v} \right\rangle$$
$$\le c \max_{\mathbf{e}\in E_K} \max_{\boldsymbol{x}\in K} \left\langle \mathbf{e}, \left| H_u(\boldsymbol{x}) \right| \mathbf{e} \right\rangle$$

- The matrix of second derivatives (known as the Hessian) is:

$$H_u(\boldsymbol{x}) = \begin{bmatrix} \frac{\partial^2 u}{\partial x^2} & \frac{\partial^2 u}{\partial x \partial y} & \frac{\partial^2 u}{\partial x \partial z} \\ \cdot & \frac{\partial^2 u}{\partial y^2} & \frac{\partial^2 u}{\partial y \partial z} \\ \cdot & \cdot & \frac{\partial^2 u}{\partial z^2} \end{bmatrix}$$

- The interpolation error in element *K* is monitored through
  - the values of the second derivatives
  - and the mesh size

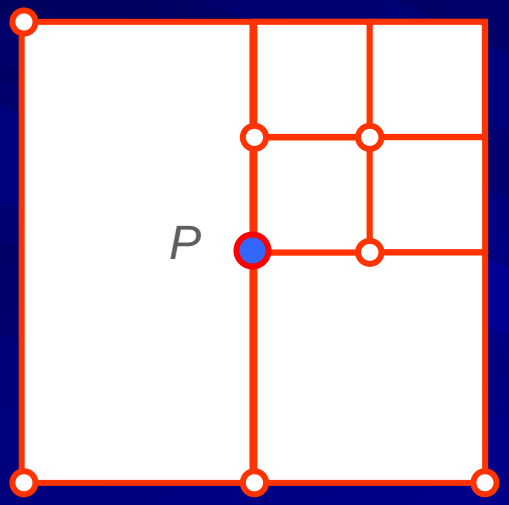
Simple geometrical considerations !!!!
Independent of the PDE !!!

Hessian-based h-adaptivity

- Last tricksy (LORT) thing: how to estimate the second derivatives …
- The Hessian at point *P* is evaluated <u>numerically</u> as follows:
  - Write a Taylor series expansion for any vertex P_i in the neighborhood of *P*

$$u(P_i) = u(P) + \overrightarrow{PP_i} \cdot \overrightarrow{\nabla u}(P) + \tfrac{1}{2}\left\langle \overrightarrow{PP_i}, \mathcal{H}_u(P)\overrightarrow{PP_i} \right\rangle + \ldots$$

  - choose P_i as the 1st and 2nd nearest neighbors of point *P, e.g.,*

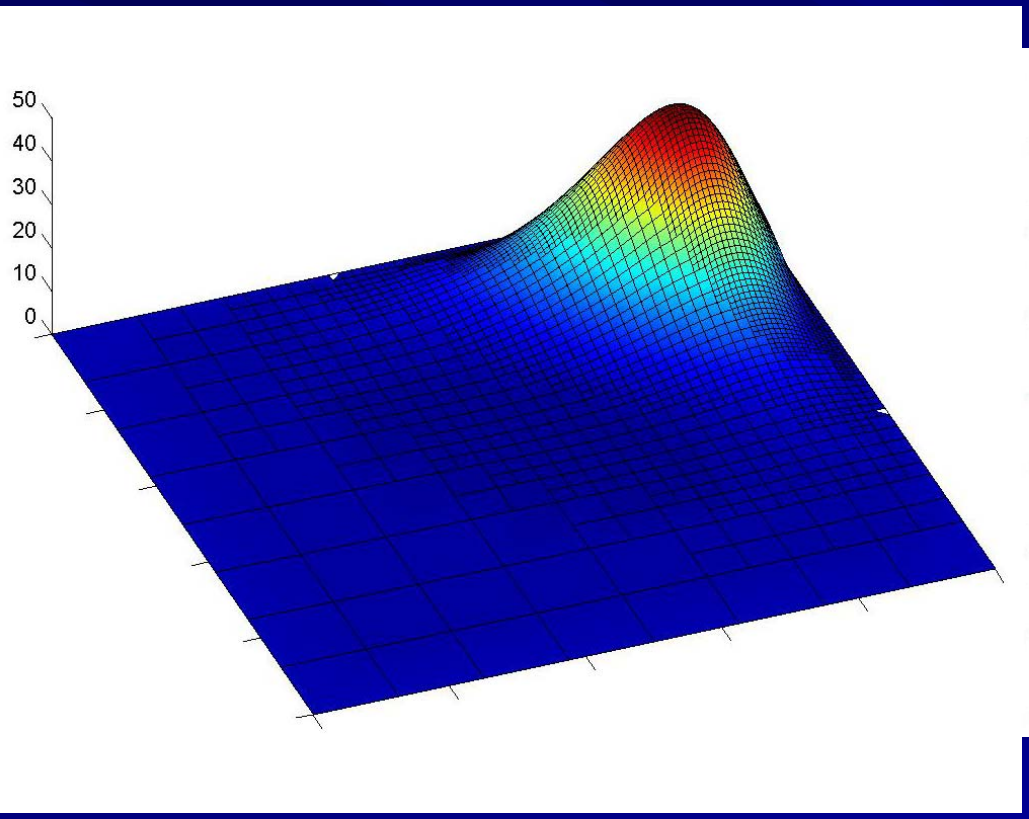


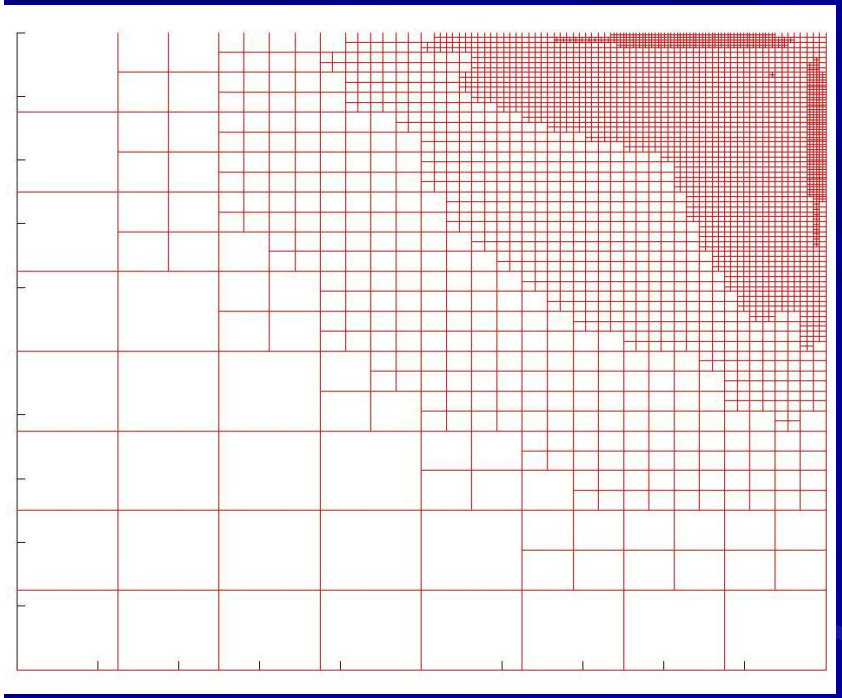
$$\mathcal{H}_u(\boldsymbol{x}) = \begin{bmatrix} a & d & e \\ d & b & f \\ e & f & c \end{bmatrix}$$

  - → an over-determined system (more neighbors than elements of matrix $\mathcal{H}_u$) (3 unknowns in 2-D and 6 unknowns in 3-D).
  - the resulting linear system is solved by a standard mean square root technique.

Hessian-based h-adaptivity: pretty pix

- 8x8 assembly, 2-g diffusion equation with X-S representative of a MSLB accident (sym. peaked solution near the boundaries)
- 4 adaptations





Hessian-based h-adaptivity

Adaptation number	# of faces	# of edges	# of vertices	# of vertices for a uniform mesh composed of the smallest size elements of the adapted mesh
Initial mesh	64	144	81	81
1	199	430	232	256
2	568	120	636	1024
3	164	3431	1778	4096
4	3340	7305	3751	16384

Comparison of geometric data between adapted grids and uniformly refined grids

- ~77% fewer vertices

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   3. Error jump-based (h-adaptivity, multi-D , diffusion **and** SPN)

B. **Goal oriented** adaptivity:
   1. Projection-based interpolation (hp-adaptivity in 1D, diffusion)

Error jump-based adaptivity

- For a very simple elliptic equation (the Poisson equation: $\Delta u = -f$), it has been proven that the jump in the solution gradient across the cell edges (or faces in 3D) is a reliable error estimator.
- For governing equations containing a Laplace operator, the Kelly error estimate has been proven to be a reliable quantification of the error.

$$\begin{aligned}
\eta_{n,g,K} &= \sqrt{h_K}\,\|[\mathbf{n}\cdot\nabla F_n^g]\|_{\partial K} \\
&= \text{error estimate for the } g\text{-th group, } n\text{-th moment flux component in cell } K \\
K &\in T_n^g \text{ is a cell of the mesh for the } g\text{-th group, } n\text{-th moment flux component}
\end{aligned}$$

- Refinement criterion:

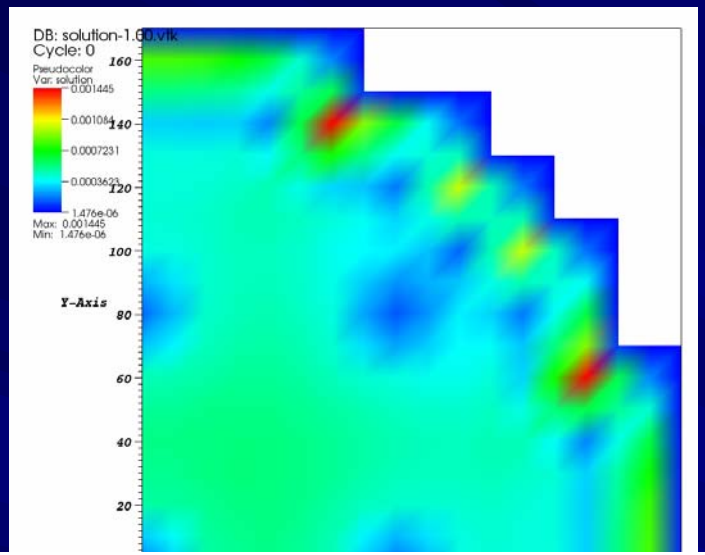
$$\eta_{n,g,K} > \alpha_1 \max_{\substack{1\le g\le G \\ 1\le n\le N \\ K\in T_n^g}} \eta_{n,g,K}$$

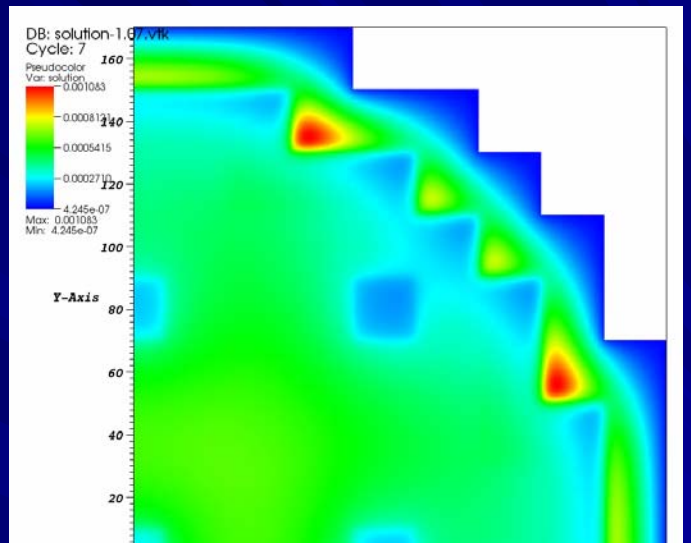
- Coarsening criterion :

$$\eta_{n,g,K} < \alpha_2 \max_{\substack{1\le g\le G \\ 1\le n\le N \\ K\in T_n^g}} \eta_{n,g,K}$$

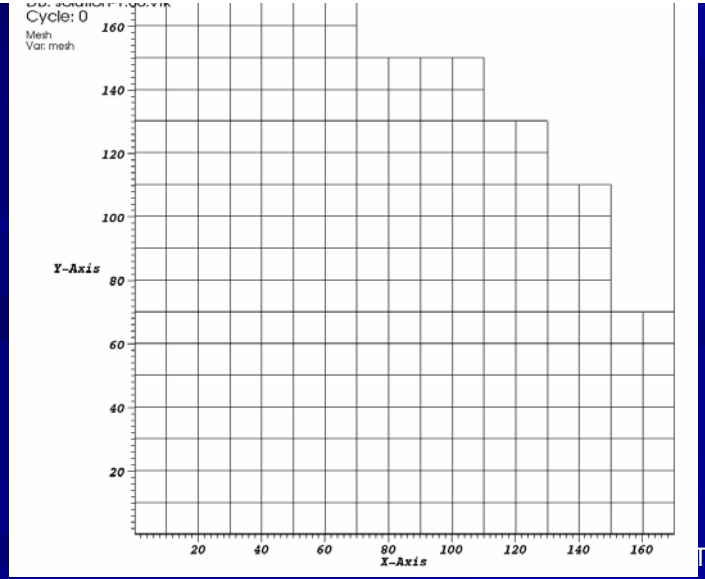
Multi-D: mesh-refinement for multigroup diffusion

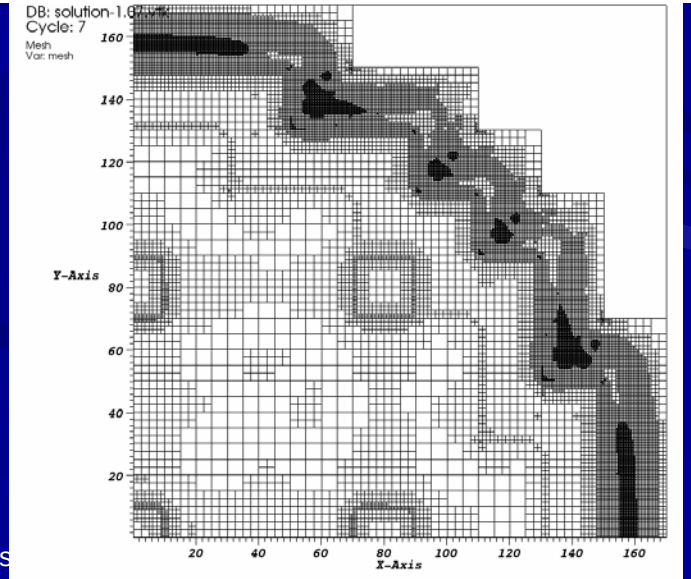
- IAEA 2D benchmark solved using 2-g diffusion:





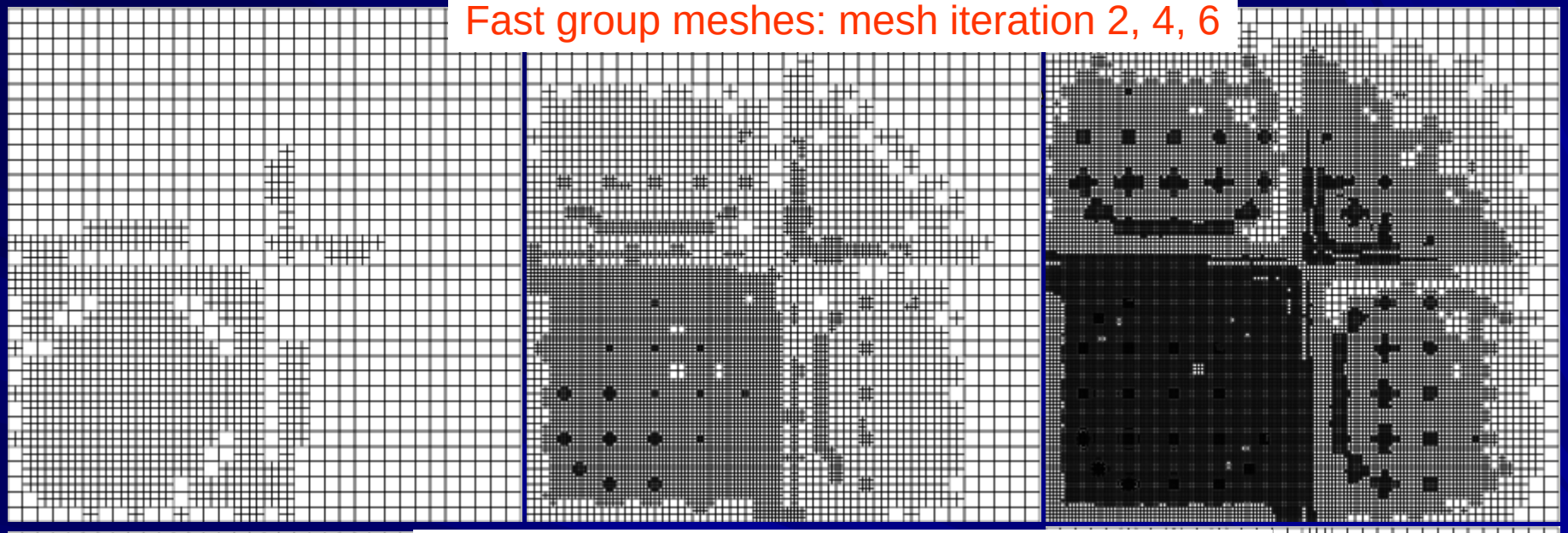
Thermal flux on the initial mesh (left) and at mesh iteration #8 (right)

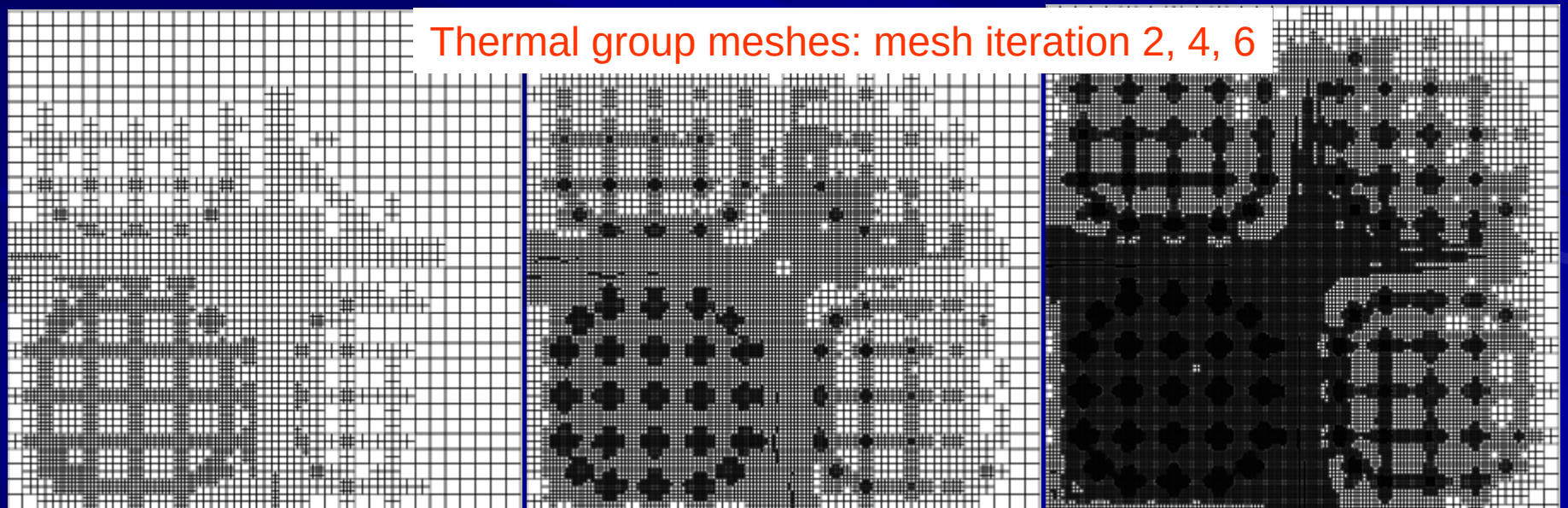




Multi-D: mesh-refinement for multigroup diffusion

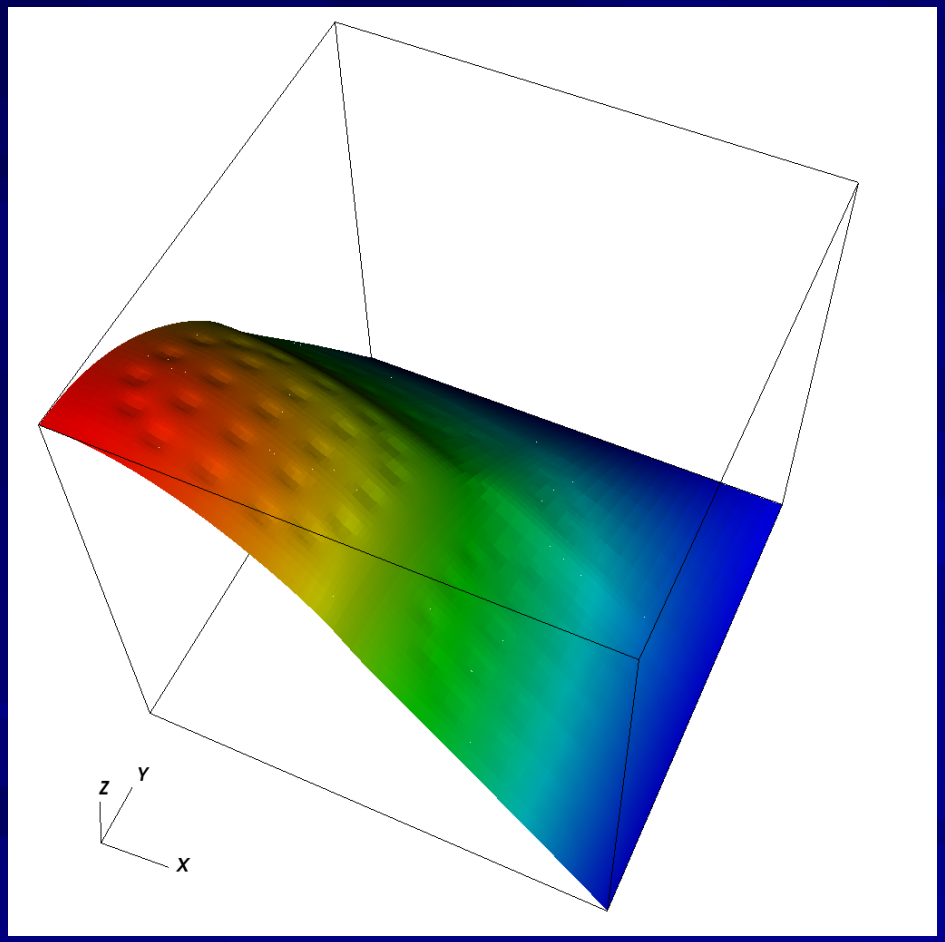
- 2-g NEA-LUOX/MOX benchmark (NEACRP-L-336)

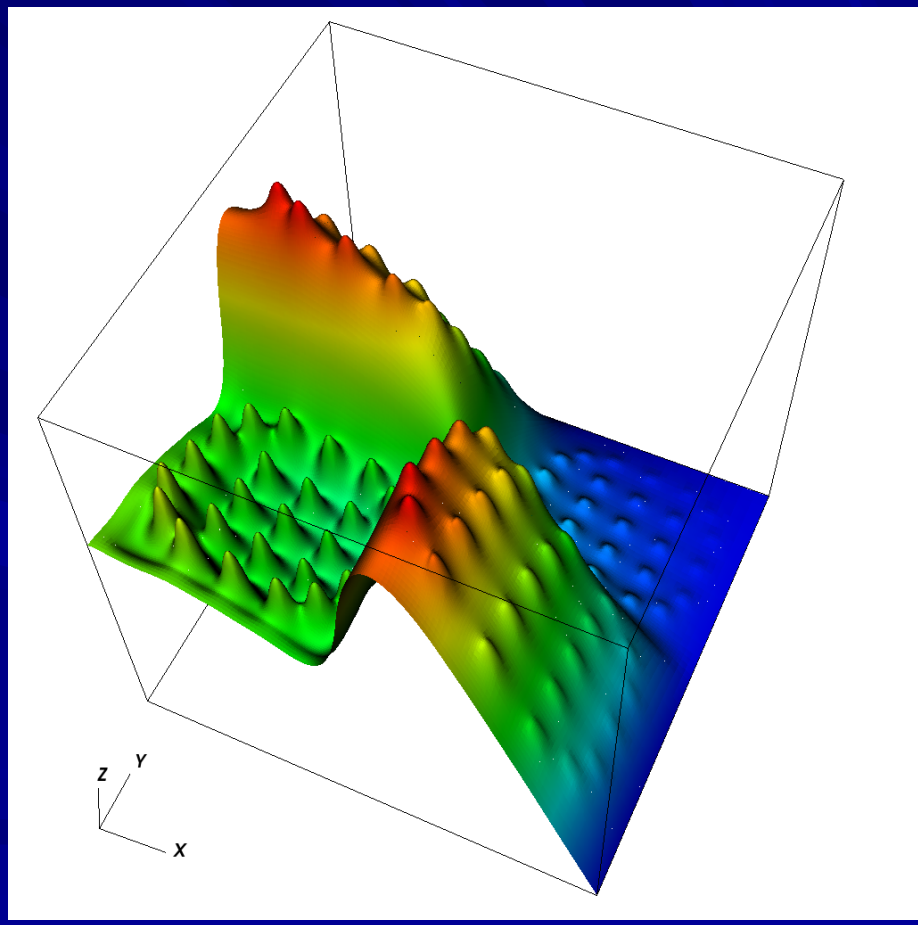




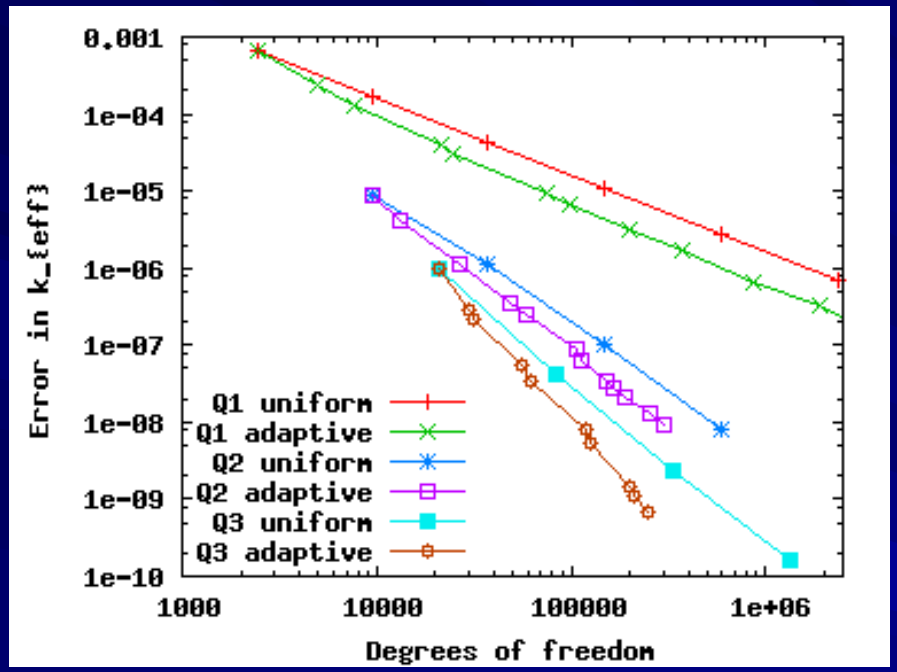
Multi-D: mesh-refinement for multigroup diffusion

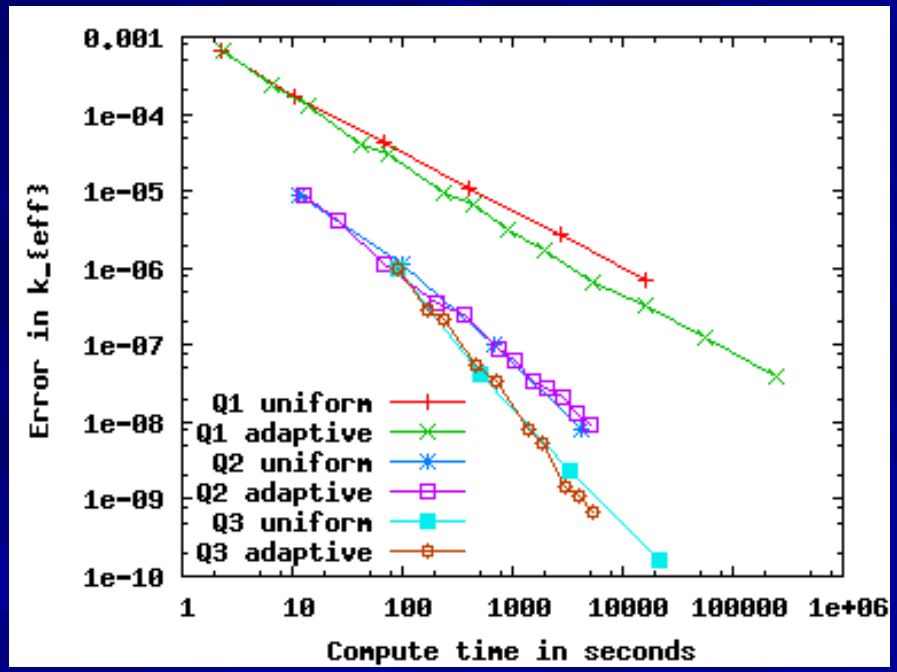
- 2-g NEA-LUOX/MOX benchmark (NEACRP-L-336)
- fast flux solution thermal flux solution





Multi-D: mesh-refinement for multigroup diffusion





Extension to multi-D multigroup SPN equations

- Simplified PN (SPN) transport equations can be recast into a system of coupled diffusion-like equations

- → Possibility to re-use all the diffusion mesh adaptivity technology to SPN equations !!!

SPN equations: Conventional formulation (1/4)

- In 1-D PN transport, the angular flux is expanded on a Legendre basis:

$$\Psi(x,\mu) = \sum_{\ell=0}^{\infty} \frac{2\ell+1}{2} \phi_\ell(x) P_\ell(\mu) \text{ with } \phi_\ell(x) = \int_{-1}^{1} d\mu \Psi(x,\mu) P_\ell(\mu)$$

- The 1-D multigroup PN equations are:

$$\frac{n}{2n+1}\frac{d\phi_{n-1}(x)}{dx} + \frac{n+1}{2n+1}\frac{d\phi_{n+1}(x)}{dx} + \sigma_{t,n}\phi_n(x) = s_n(x)\delta_{n0} \text{ for any } 0 \le n \le N$$

  - With $\sigma_{t,m} = \sigma - \sigma_{s,m}\ .\ 0 \le m \le N$ a (possibly full) matrix of size GxG
  - Any vector (flux or source) is of length G
  - The external source was assumed isotropic

SPN equations: Conventional formulation (2/4)

- Defining

$$\boldsymbol{\phi} = \begin{bmatrix} \phi_0 \\ \phi_1 \\ \phi_2 \\ \vdots \\ \vdots \\ \phi_{N-1} \\ \phi_N \end{bmatrix} \quad \text{and } \mathbf{s} = \begin{bmatrix} s_0 \\ 0 \\ \\ \vdots \\ \vdots \\ \\ 0 \end{bmatrix}$$

$$\begin{aligned} C &= diag(\sigma_{t,0}, \sigma_{t,1}, \cdots, \sigma_{t,N-1}, \sigma_{t,N}) \\ A &= \begin{bmatrix} 0 & 1 & & & & & \\ 1/3 & 0 & 2/3 & & & & \\ & 2/5 & 0 & 3/5 & & & \\ & & \ddots & 0 & \ddots & & \\ & & & \ddots & 0 & \ddots & \\ & & & & \frac{N-1}{2N-1} & 0 & \frac{N}{2N-1} \\ & & & & & \frac{N}{2N+1} & 0 \end{bmatrix} \end{aligned}$$

the 1-D multigroup PN equations are:

$$\boxed{A\frac{d\boldsymbol{\phi}}{dx} + C\boldsymbol{\phi} = \mathbf{s} + \mathrm{BC}}$$

- Elimination of the odd moments from the odd equations and substitution into the even equations yields

$$\begin{aligned} & -\frac{n}{2n+1}\frac{d}{dx}\left[\sigma_{t,n-1}^{-1}\left[\frac{n-1}{2n-1}\frac{d\phi_{n-2}(x)}{dx} + \frac{n}{2n-1}\frac{d\phi_n(x)}{dx}\right]\right] \\ & -\frac{n+1}{2n+1}\frac{d}{dx}\left[\sigma_{t,n+1}^{-1}\left[\frac{n+1}{2n+3}\frac{d\phi_n(x)}{dx} + \frac{n+2}{2n+3}\frac{d\phi_{n+2}(x)}{dx}\right]\right] \\ +\sigma_{t,n}\phi_n(x) \quad = \quad & s_n(x)\delta_{n,0} \text{ for any } 0 \le n \le N-1 \text{ and } n \textbf{ EVEN} \end{aligned}$$

SPN equations: Conventional formulation (3/4)

- Multi-D equations are obtained formally by replacing

$$\frac{d}{dx}\sigma_t^{-1}\frac{d\phi}{dx} \text{ by } \nabla \cdot \sigma_t^{-1}\nabla\phi$$

- Defining composite moments as follows concludes the derivation

$$F_n \equiv (n+1)\phi_n + (n+2)\phi_{n+2} \text{ for any } 0 \leq n \leq N-1 \text{ and } n \textbf{ EVEN}$$

SPN equations: Conventional formulation (4/4)

- Example: SP7

$$-\nabla\cdot\frac{1}{3}\sigma_{t,1}^{-1}\nabla F_0+\sigma_{t,0}F_0=s_0+\frac{2}{3}\sigma_{t,0}F_2-\frac{8}{15}\sigma_{t,0}F_4+\frac{16}{35}\sigma_{t,0}F_6$$

$$-\nabla\cdot\frac{1}{7}\sigma_{t,3}^{-1}\nabla F_2+\left(\frac{4}{9}\sigma_{t,0}+\frac{5}{9}\sigma_{t,2}\right)F_2=-\frac{2}{3}s_0+\frac{2}{3}\sigma_{t,0}F_0+\left(\frac{16}{45}\sigma_{t,0}+\frac{4}{9}\sigma_{t,2}\right)F_4-\left(\frac{32}{105}\sigma_{t,0}+\frac{8}{21}\sigma_{t,2}\right)F_6$$

$$\begin{aligned}-\nabla\cdot\frac{1}{11}\sigma_{t,5}^{-1}\nabla F_4+\left(\frac{64}{225}\sigma_{t,0}+\frac{16}{45}\sigma_{t,2}+\frac{9}{25}\sigma_{t,4}\right)F_4 &= \frac{8}{15}s_0-\frac{8}{15}\sigma_{t,0}F_0+\left(\frac{16}{45}\sigma_{t,0}+\frac{4}{9}\sigma_{t,2}\right)F_2\\ &\quad+\left(\frac{128}{525}\sigma_{t,0}+\frac{32}{105}\sigma_{t,2}+\frac{54}{175}\sigma_{t,4}\right)F_6\end{aligned}$$

$$\begin{aligned}-\nabla\cdot\frac{1}{15}\sigma_{t,7}^{-1}\nabla F_6+\left(\frac{256}{1225}\sigma_{t,0}+\frac{64}{245}\sigma_{t,2}+\frac{324}{1225}\sigma_{t,4}+\frac{13}{49}\sigma_{t,6}\right)F_6 &= -\frac{16}{35}s_0+\frac{16}{35}\sigma_{t,0}F_0\\ &\quad-\left(\frac{32}{105}\sigma_{t,0}+\frac{8}{21}\sigma_{t,2}\right)F_2\\ &\quad+\left(\frac{128}{525}\sigma_{t,0}+\frac{32}{105}\sigma_{t,2}+\frac{54}{175}\sigma_{t,4}\right)F_4\end{aligned}$$

SPN equations: Alternative formulation (1/3)

- Using the fact that the Legendre basis is orthogonal, the angular flux is expanded as

$$\Psi(x,\mu) \equiv \sum_{\ell=0}^{\infty} \alpha_\ell \phi_\ell(x) P_\ell(\mu)$$

- The coefficients α_ℓ are chosen so that matrix *A* is as simple as possible to allow easy elimination/substitution of the odd moments.
- The choice of coefficients is

$$\begin{aligned} \alpha_0 &= 1 \\ \alpha_m &= \frac{4m^2-1}{m\alpha_{m-1}} \end{aligned}$$

- Performing the elimination/substitution of the odd moments and defining composite moments as follows concludes the derivation

$$F_n \equiv \phi_n + \phi_{n+2} \text{ for any } 0 \le n \le N-1 \text{ and } n \textbf{ EVEN}$$

SPN equations: Alternative formulation (2/3)

- Relationship between the moments and composite moments:

$$F = \begin{bmatrix} F_0 \\ \\ \\ F_{N-1} \end{bmatrix} = \begin{bmatrix} 1 & 1 & & & \\ & 1 & 1 & & \\ & & 1 & 1 & \\ & & & 1 & 1 \\ & & & & 1 \end{bmatrix} \begin{bmatrix} \phi_0 \\ \phi_2 \\ \vdots \\ \phi_{N-3} \\ \phi_{N-1} \end{bmatrix} = C_1 \cdot \Phi_e$$

$$\Phi_e = C_1^{-1} \cdot F = \begin{bmatrix} 1 & -1 & +1 & -1 & +1 \\ & 1 & -1 & 1 & -1 \\ & & 1 & -1 & 1 \\ & & & 1 & -1 \\ & & & & 1 \end{bmatrix} \cdot F$$

- Final set of coupled diffusion-like SPN equations

$$\boxed{\left[C_2 \cdot \partial_{xx} \circ + D_e C_1^{-1}\right] \cdot F = s_e}$$

  – with

$$C_2 = -C_1^T D_o^{-1}$$

$$D_e = diag\left[\sigma_{t,0} \quad \sigma_{t,2} \quad \sigma_{t,4} \quad \cdots \quad \sigma_{t,N-3} \quad \sigma_{t,N-1}\right]$$

$$s_e = \begin{bmatrix} s_0 \\ 0 \\ \vdots \\ 0 \end{bmatrix}$$

SPN equations: Alternative formulation (3/3)

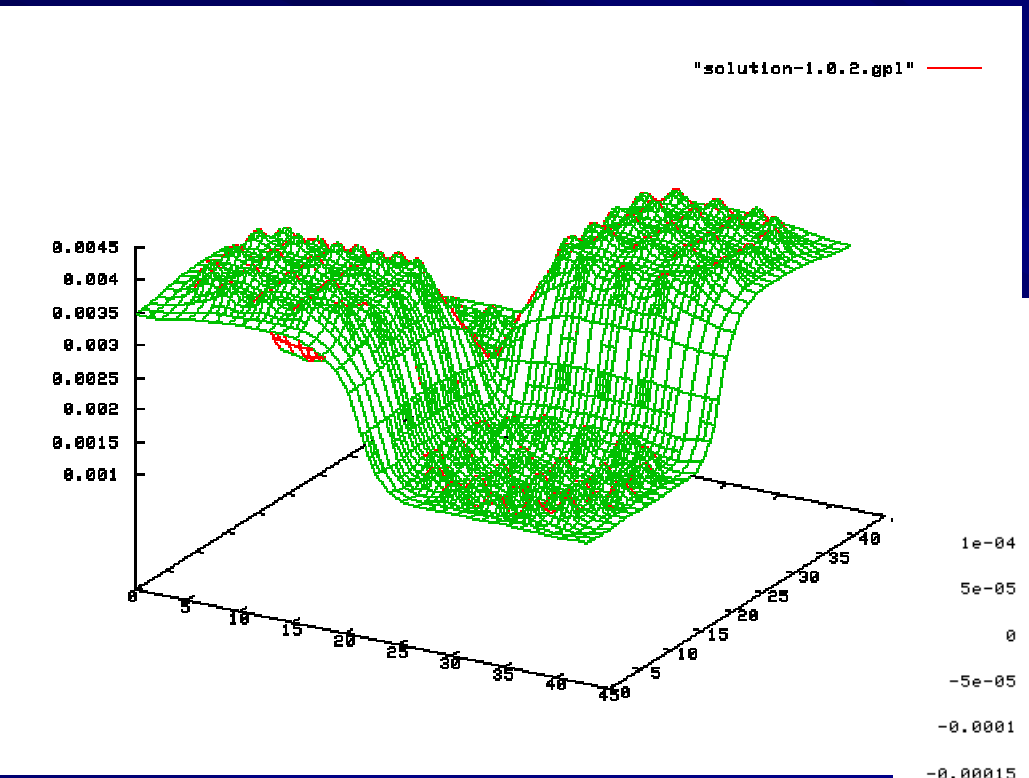
- Example: SP7

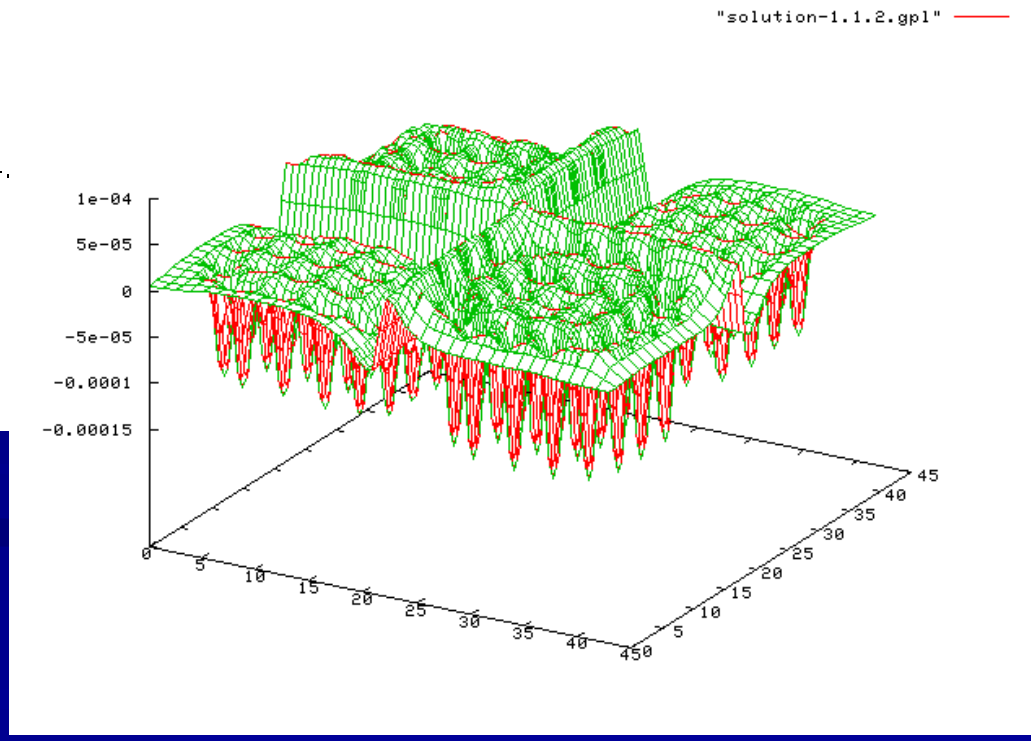
$$
\begin{aligned}
-\nabla\cdot\sigma_{t,1}^{-1}\nabla F_0+\sigma_{t,0}F_0 &= +s_0+\sigma_{t,0}\left(F_2-F_4+F_6\right)\\
-\nabla\cdot\sigma_{t,3}^{-1}\nabla F_2+\left(\sigma_{t,0}+\sigma_{t,2}\right)F_2 &= -s_0+\sigma_{t,0}F_0+\left(\sigma_{t,0}+\sigma_{t,2}\right)F_4-\left(\sigma_{t,0}+\sigma_{t,2}\right)F_6\\
-\nabla\cdot\sigma_{t,5}^{-1}\nabla F_4+\left(\sigma_{t,0}+\sigma_{t,2}+\sigma_{t,4}\right)F_4 &= +s_0-\sigma_{t,0}F_0+\left(\sigma_{t,0}+\sigma_{t,2}\right)F_2+\left(\sigma_{t,0}+\sigma_{t,2}+\sigma_{t,4}\right)F_6\\
-\nabla\cdot\sigma_{t,7}^{-1}\nabla F_6+\left(\sigma_{t,0}+\sigma_{t,2}+\sigma_{t,4}+\sigma_{t,6}\right)F_6 &= -s_0+\sigma_{t,0}F_0-\left(\sigma_{t,0}+\sigma_{t,2}\right)F_2+\left(\sigma_{t,0}+\sigma_{t,2}+\sigma_{t,4}\right)F_4
\end{aligned}
$$

- Simpler coefficients, more amenable coding and generalization to any N order.

Multi-D: mesh-refinement for multigroup **SPN** transport

- 2-g UOX/MOX benchmark (reflective BC):
- Shown: moments 0 and 2 of the thermal flux (**SP3** calculation)

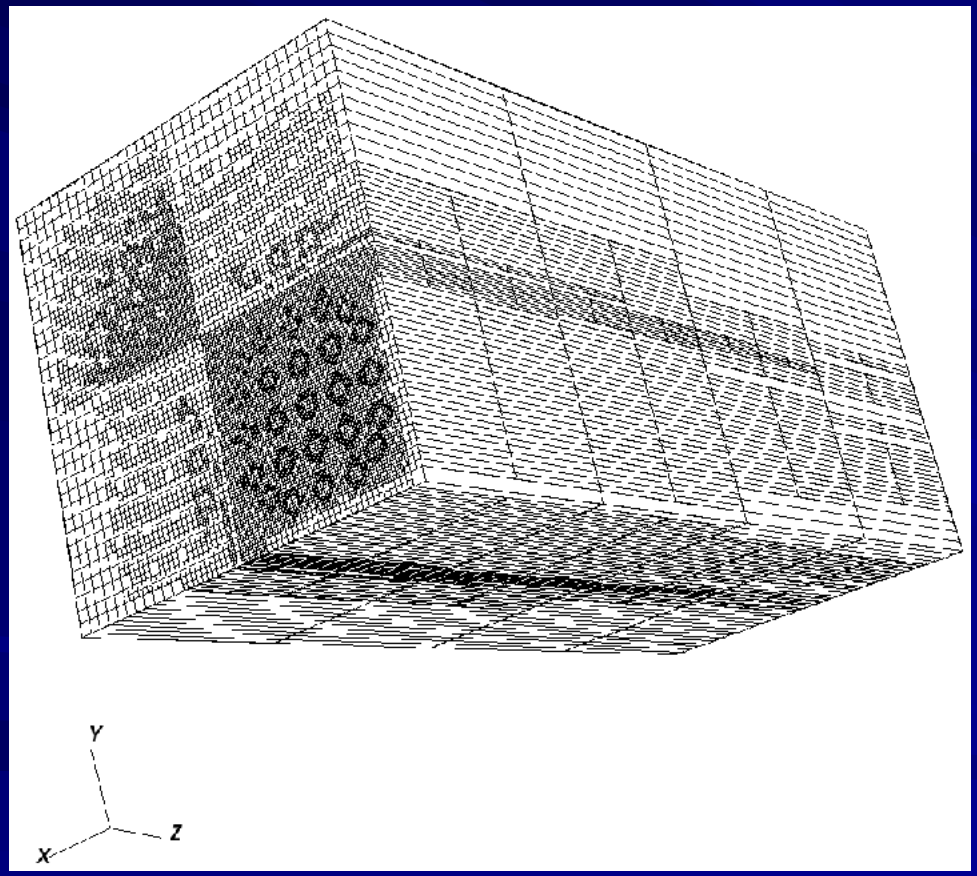


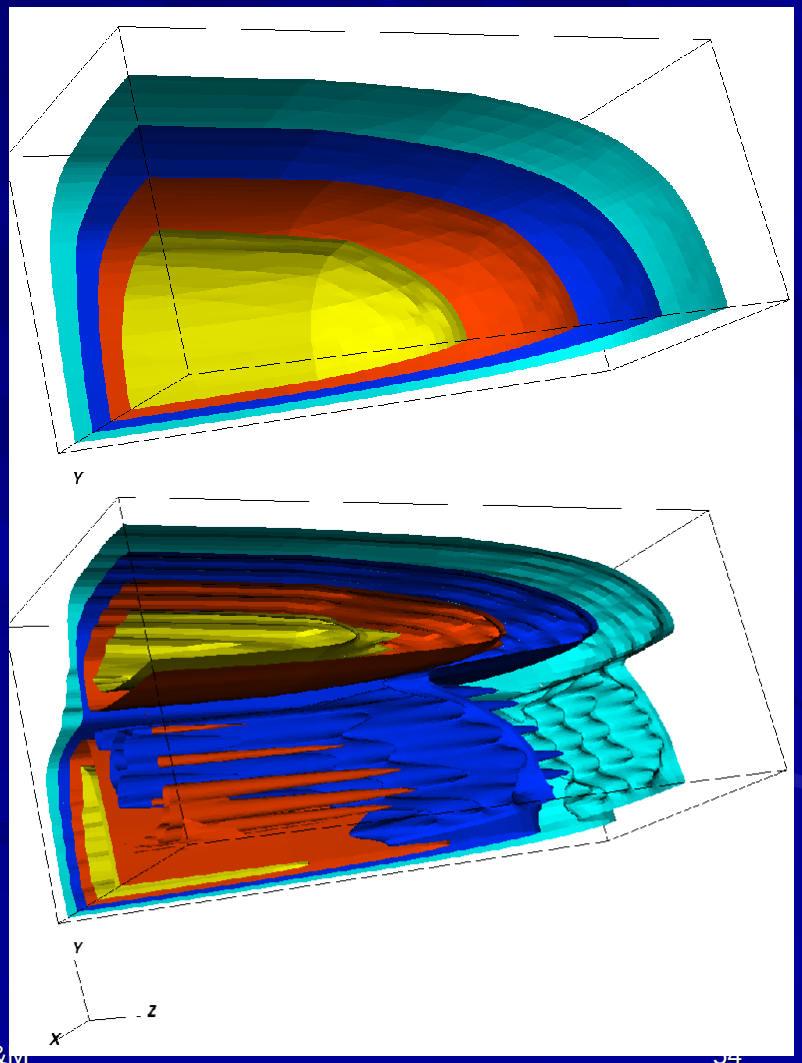


Magnitude is decreasing with moments

Multi-D: mesh-refinement for multigroup **SPN** transport

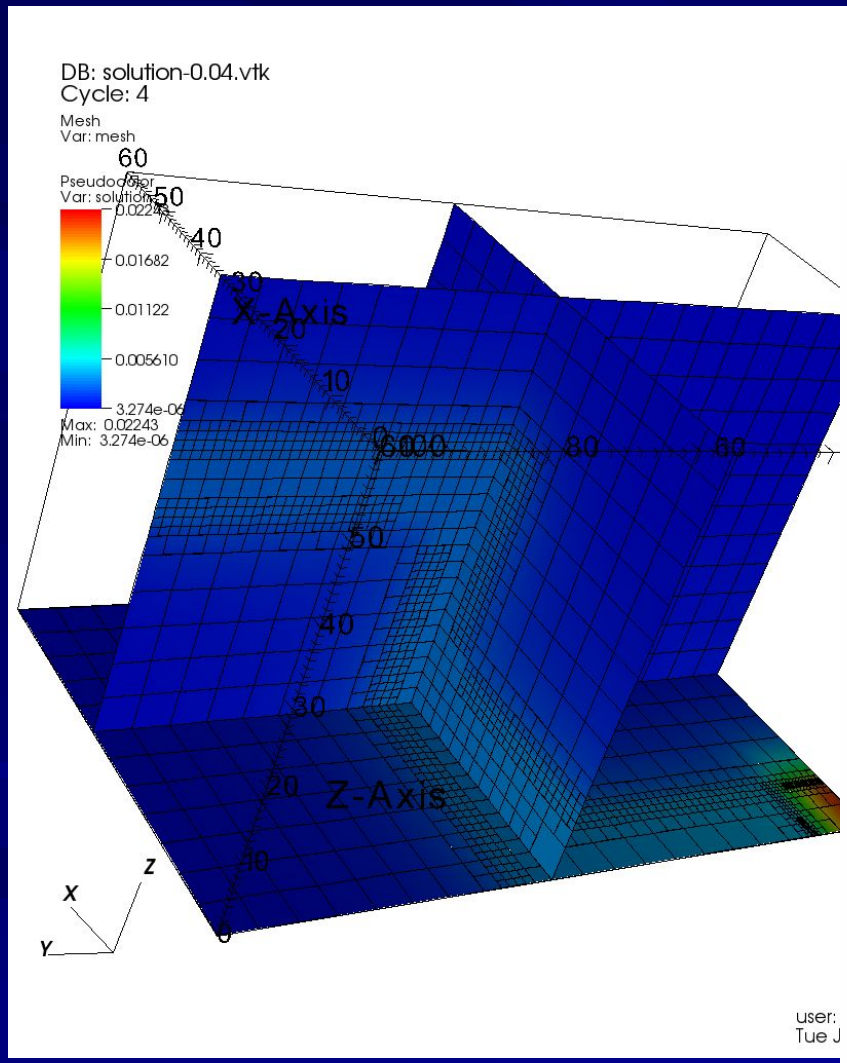
- 2-g UOX/MOX benchmark (3D extension)
- Shown: moments 0 of the fast and thermal flux (**SP3** calculation) and moment 0 thermal mesh

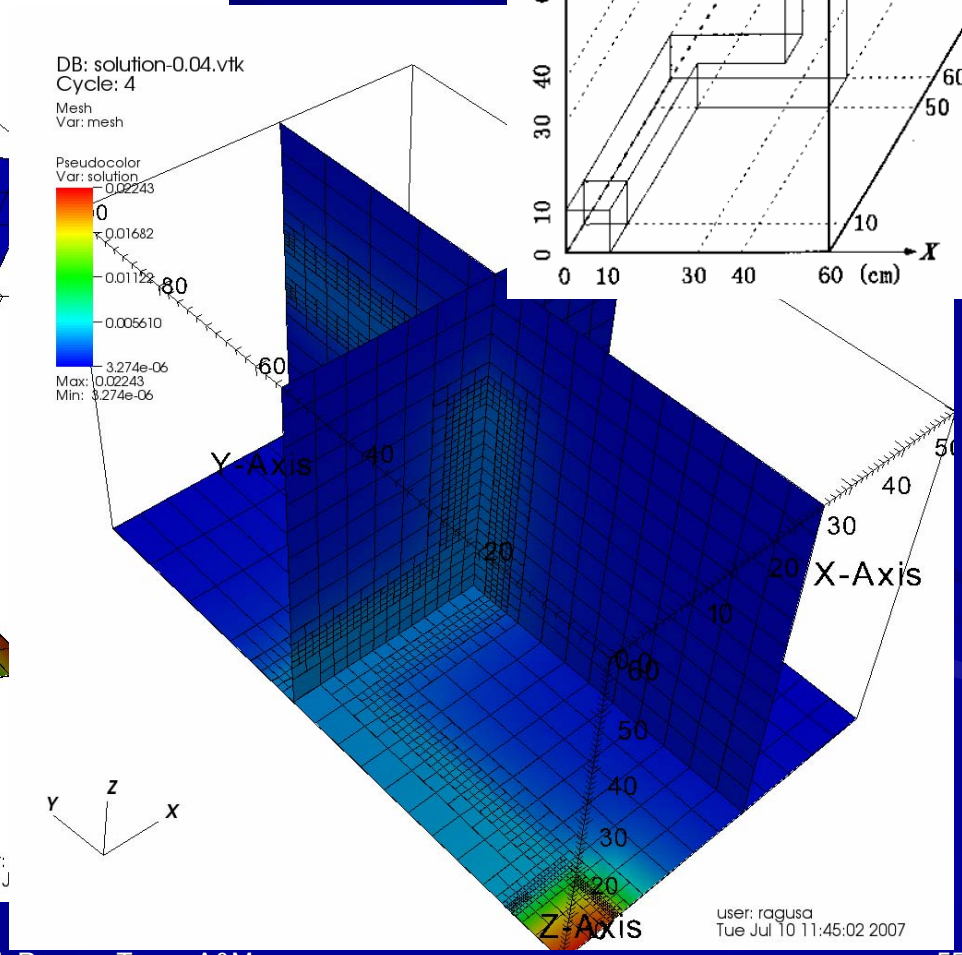


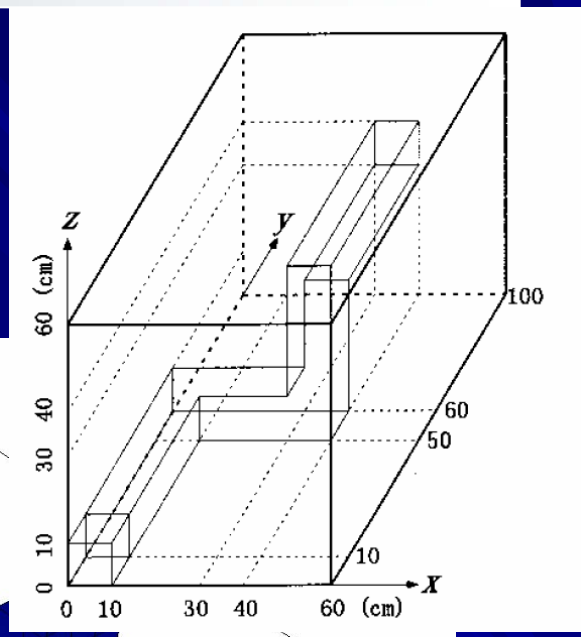


Multi-D: mesh-refinement for multigroup **SPN** transport

- Kobayashi, *modified* problem #3 (SP5 results).







Mesh adaptation applications: MG diffusion / SPN

- Multigroup Diffusion and Simplified PN Transport (SPN) equations
- Ongoing work : Multigroup SN Transport equations

- Application examples:

A. **Standard** adaptivity with 3 different error estimates:
   1. Projection-based interpolation (hp-adaptivity in 1D, diffusion)
   2. Hessian-based (h-adaptivity, multi-D , diffusion)
   3. Error jump-based (h-adaptivity, multi-D , diffusion **and** SPN)

B. **Goal oriented** adaptivity:
   1. Projection-based interpolation (hp-adaptivity in 1D, diffusion)

Goal-Oriented hp-technology

- Combines the properties of hp-adaptivity with **goal-oriented** calculations

- Why?
  - We do not necessarily want the best solution everywhere but only in localized sub-domains → **quantities of interest**

- Typical **quantities of interest**:
  - reaction rates in sub-domains
  - point-wise fluxes
  - point-wise currents
  - any linear functional of the solution

hp-Goal-Oriented : reaction rate as a Q of Interest

- Detector response (reaction rate)

$$I(\phi) = \sum_{g=1}^{G} \int_{\Omega_{\text{det}}} \Sigma_a^g(x)\phi^g(x)dx$$

- Error in the quantity of interest is given by

$$\delta_{hp} = \left| I(\phi) - I(\phi_{hp}) \right|$$

- Let us take a look at the dual (adjoint) problem
  - Adjoint source

$$Q^{g,\dagger}(x) = \begin{cases} \Sigma_a^g(x) \text{ for } x \in \Omega_{\text{det}} \\ 0 \quad \text{otherwise} \end{cases}, \qquad \forall\, g = 1, 2, \cdots, G$$

  - Adjoint variational formulation

$$b^{\dagger}(\phi^{\dagger}, \varphi) = I(\varphi) = b(\varphi, \phi^{\dagger}), \quad \forall\, \varphi \in H^1(\Omega)$$

  - Error in the quantity of interest

$$\left| I(\phi) - I(\phi_{hp}) \right| = \left| b(\phi - \phi_{hp}, \phi^{\dagger}) \right| = \left| b(e_{hp}, \phi^{\dagger}) \right|$$

- By Galerkin orthogonality,

$$\delta_{hp} = \left| I(\phi) - I(\phi_{hp}) \right| = \left| b(e_{hp}, e_{hp}^{\dagger}) \right| = \left| b(\phi - \phi_{hp}, \phi^{\dagger} - \phi_{hp}^{\dagger}) \right|$$

Error is measured in the bilinear inner product ~ H-1 norm
→ re-use all the standard hp-techniques !!!

Goal-Oriented hp- error estimates

- Goal-oriented error is given by

$$\delta_{hp} = \left| I(\phi) - I(\phi_{hp}) \right| = \left| b(e_{hp}, e_{hp}^{\dagger}) \right| = \left| b(\phi - \phi_{hp}, \phi^{\dagger} - \phi_{hp}^{\dagger}) \right|$$

- Same 'trick' as for standard hp-techniques
  - Use for fine solution $\boxed{\phi \approx \phi_{hp-fine} = \phi_{h/2,p+1}}$
  - Use for coarse solution $\boxed{\phi_{hp-coarse} = \Pi_{hp-coarse}\phi_{hp-fine} = \Pi_{hp}\phi_{h/2;p+1}}$
  - Goal-oriented error :

$$\begin{aligned}\delta_{hp} &= \left| b(\phi_{h/2,p+1} - \Pi_{hp}\phi_{h/2;p+1}, \phi_{h/2,p+1}^{\dagger} - \Pi_{hp}\phi_{h/2;p+1}^{\dagger}) \right| \\ &\leq \sum_{g=1}^{G} \sum_{K^g} \left| \phi_{h/2,p+1}^{g} - \Pi_{hp}\phi_{h/2;p+1}^{g} \right|_{1,K^g} \left| \phi_{h/2,p+1}^{g,\dagger} - \Pi_{hp}\phi_{h/2;p+1}^{g,\dagger} \right|_{1,K^g}\end{aligned}$$

  - Error indicator:

$$\mu_K^g = \left| \phi_{h/2,p+1}^{g} - \Pi_{hp}\phi_{h/2;p+1}^{g} \right|_{1,K^g} \left| \phi_{h/2,p+1}^{g,\dagger} - \Pi_{hp}\phi_{h/2;p+1}^{g,\dagger} \right|_{1,K^g}$$

hp-Goal-Oriented : Q of Interest = flux or current

- Point-wise flux
  - Adjoint source term: $$\boxed{Q^{g',\dagger}(\vec{r}) = \delta(g-g') \times \vec{n} \cdot \vec{\nabla}(D_g \delta(\vec{r}-\vec{r}_0))}$$
  - Quantity of interest functional

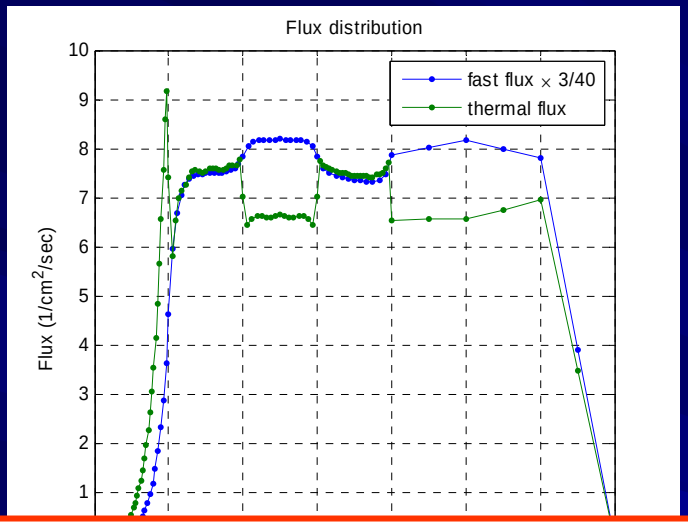
$$I(\phi) = \sum_{g'=1}^{G} (\phi^{g'}, Q^{g',\dagger}(\vec{r})) = (\phi^g, Q^{g,\dagger}(\vec{r})) = \int_\Omega d^3r \ \phi^g(\vec{r}) \vec{n} \cdot \vec{\nabla}(D_g \delta(\vec{r}-\vec{r}_0)) = \vec{J}^g(\vec{r}_0) \cdot \vec{n}$$

- Point-wise current
  - Adjoint source term: $$\boxed{Q^{g',\dagger}(\vec{r}) = \delta(g-g') \times \delta(\vec{r}-\vec{r}_0)}$$
  - Quantity of interest functional

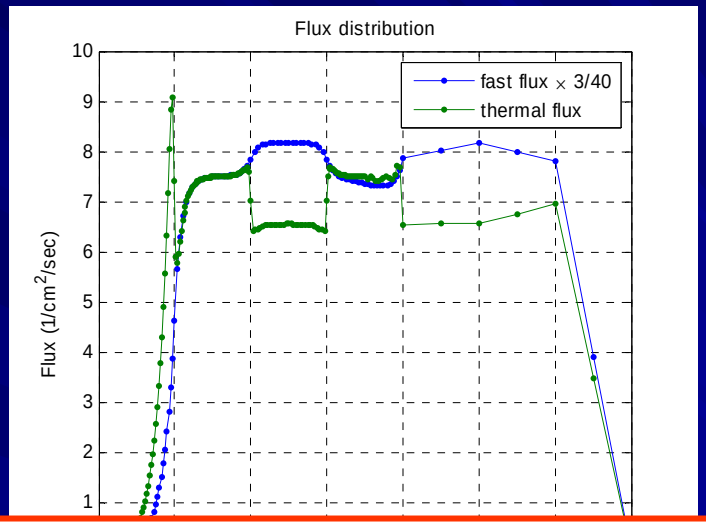
$$I(\phi) = \sum_{g'=1}^{G} (\phi^{g'}, Q^{g',\dagger}(\vec{r})) = (\phi^g, Q^{g,\dagger}(\vec{r})) = \int_\Omega d^3r \ \phi^g(\vec{r}) \delta(\vec{r}-\vec{r}_0) = \phi^g(\vec{r}_0)$$

Goal-oriented hp-Adaptive Mesh Refinement: results

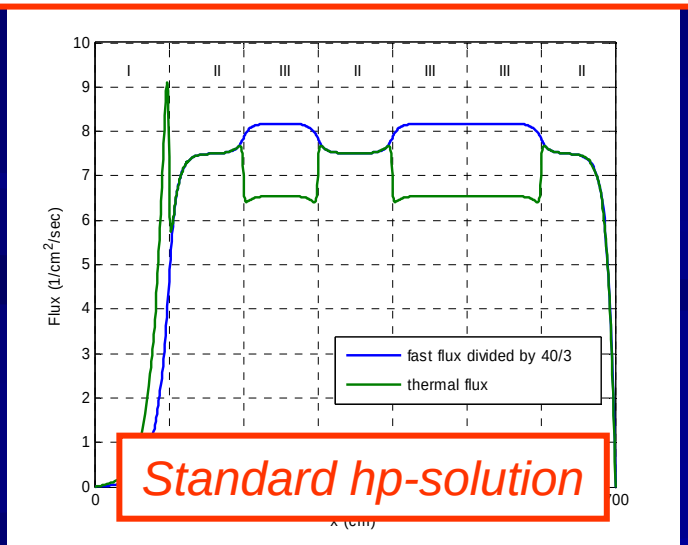
- Two-group, 7-region eigenproblem
  - Goal-oriented solution (for an accurate solution only in 100<x<300)



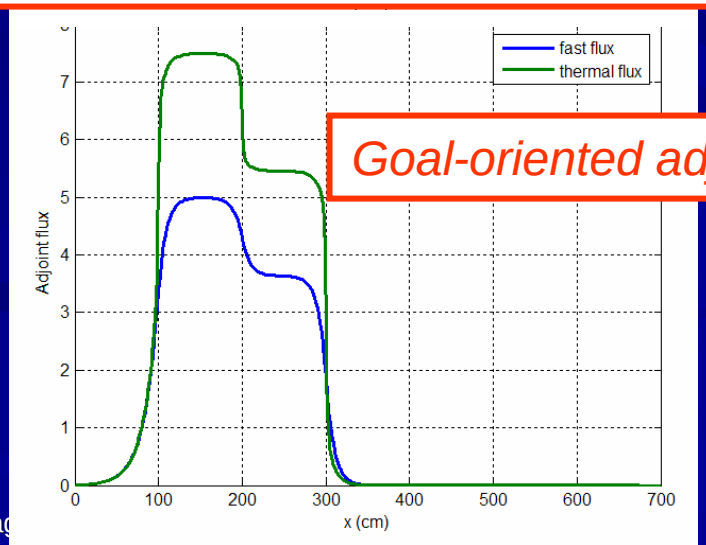
Goal-oriented hp-solution, tol=1%



Goal-oriented hp-solution, tol=0.1%



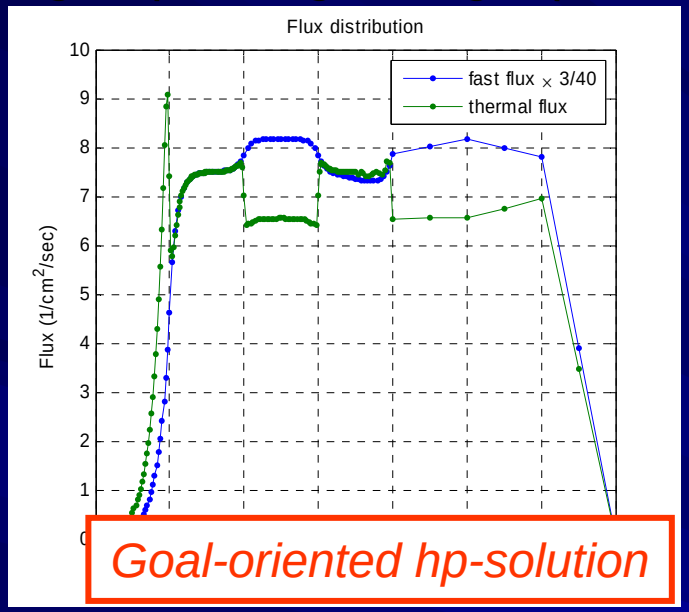
Standard hp-solution

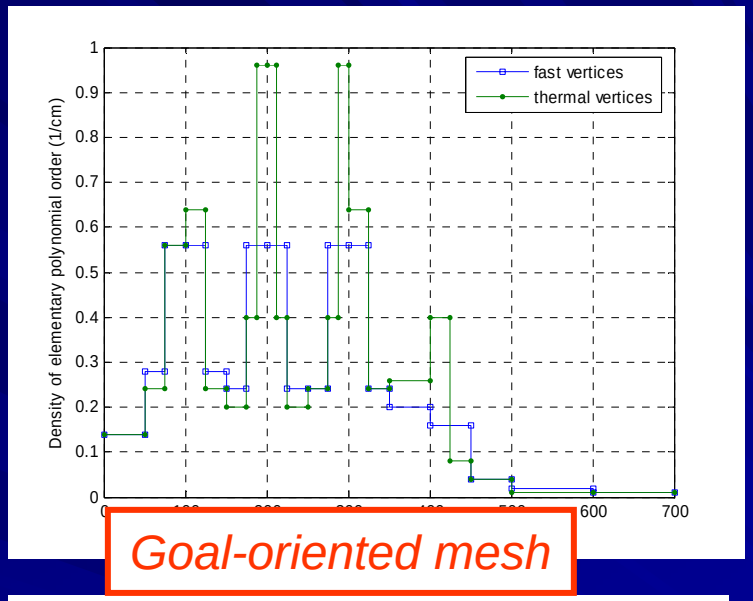


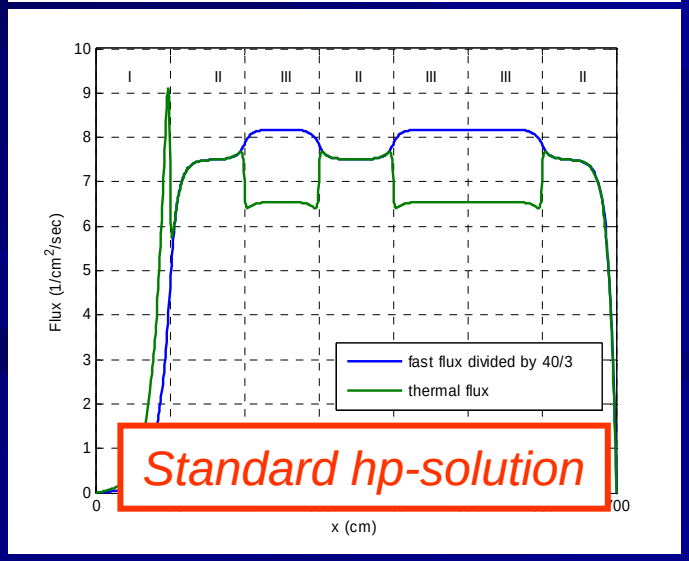
Goal-oriented adjoint flux

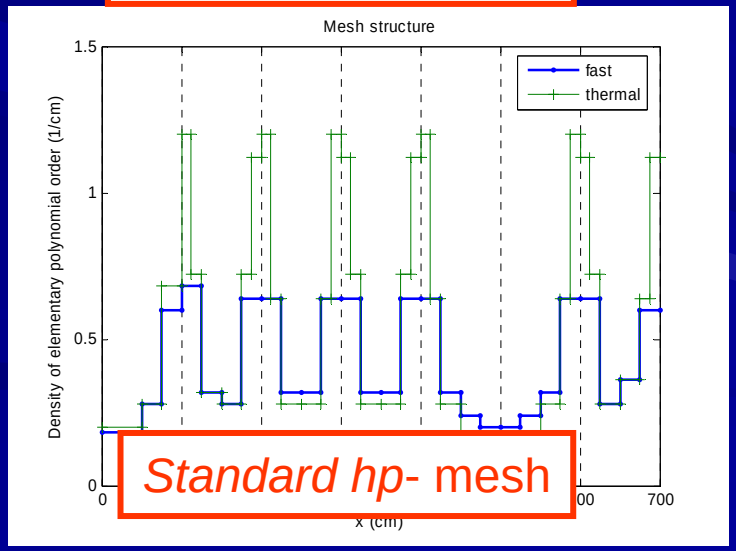
Goal-oriented hp-Adaptive Mesh Refinement: results

- Two-group, 7-region eigenproblem





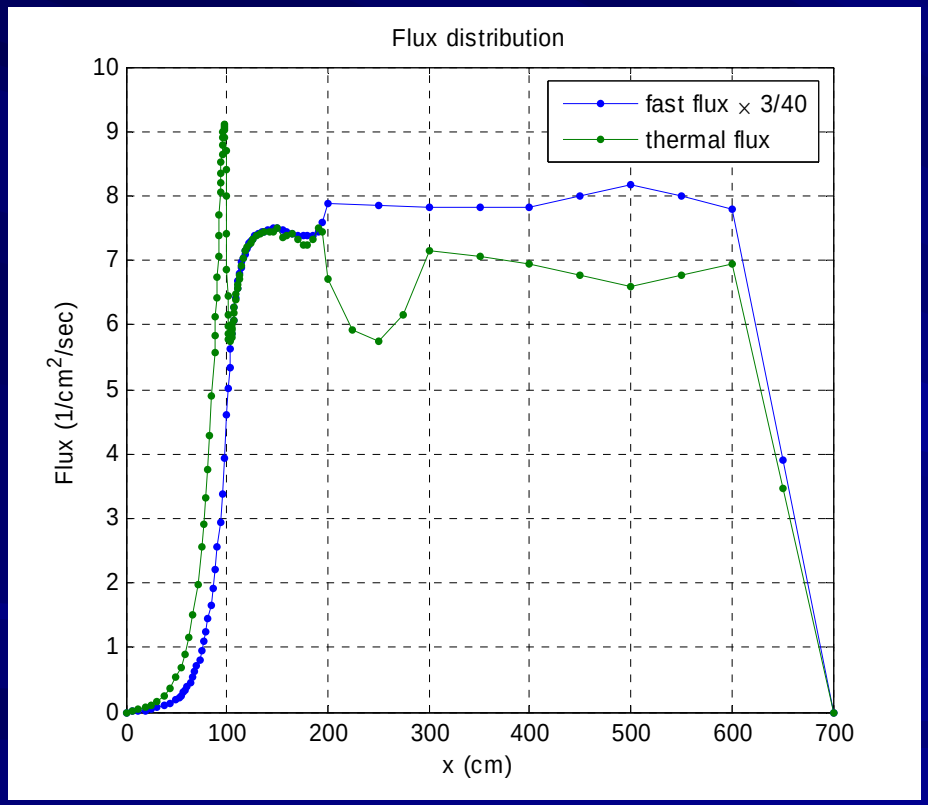




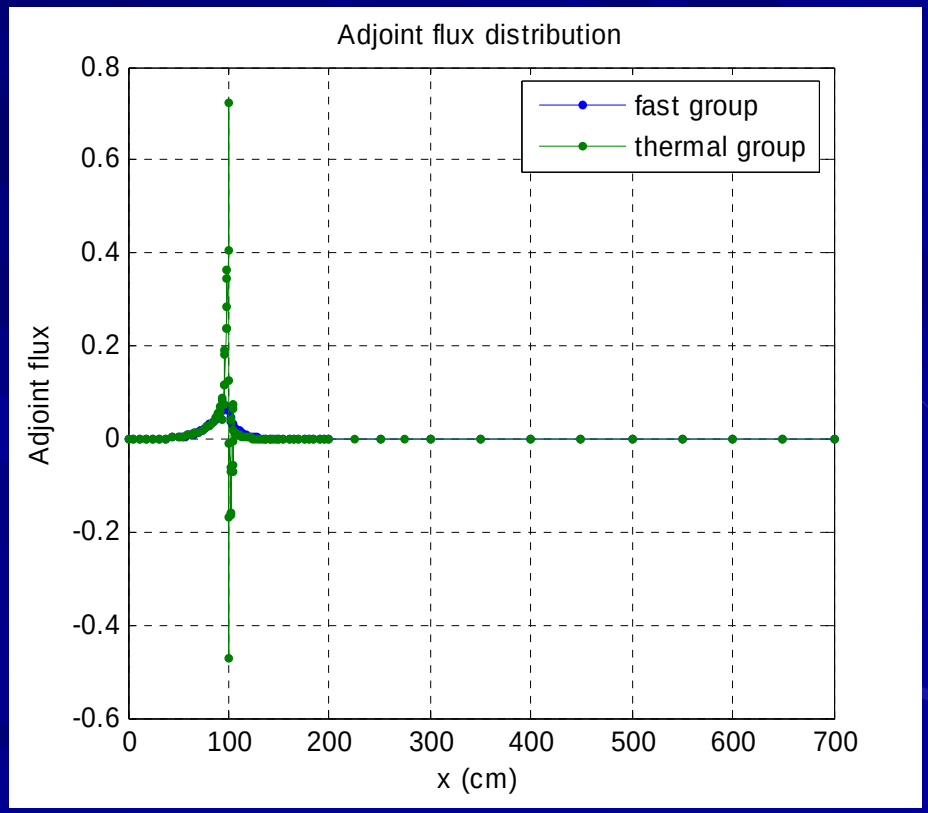
Goal-oriented hp-Adaptive Mesh Refinement: results

- GOAL: Point-wise current at x= 100

Goal-oriented hp-solution, tol=1%



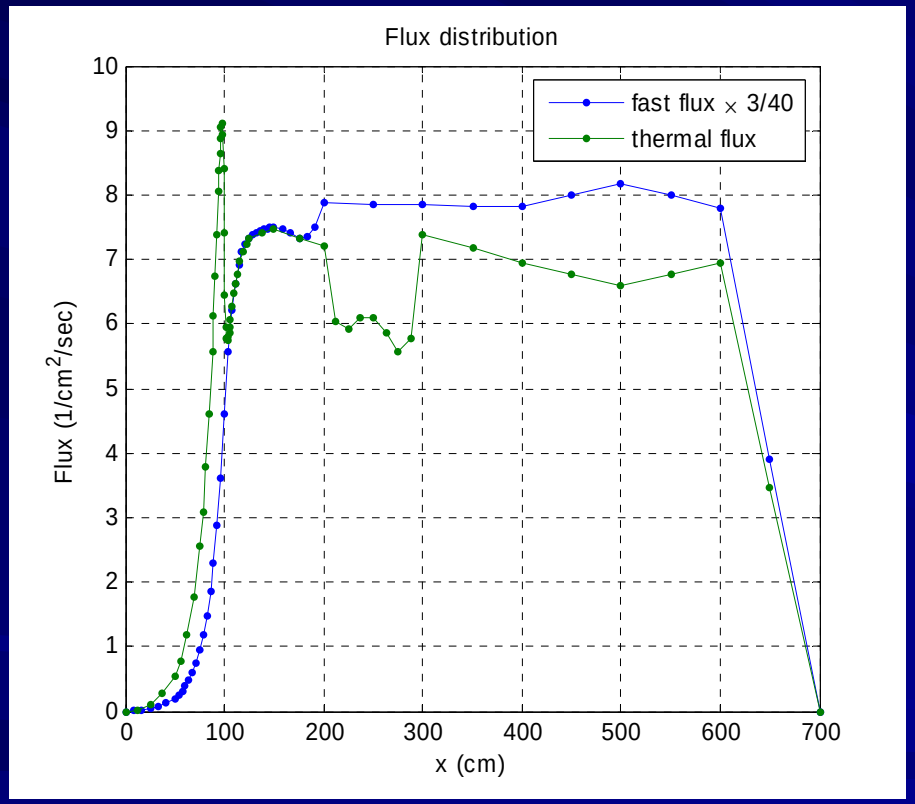
Goal-oriented adjoint flux



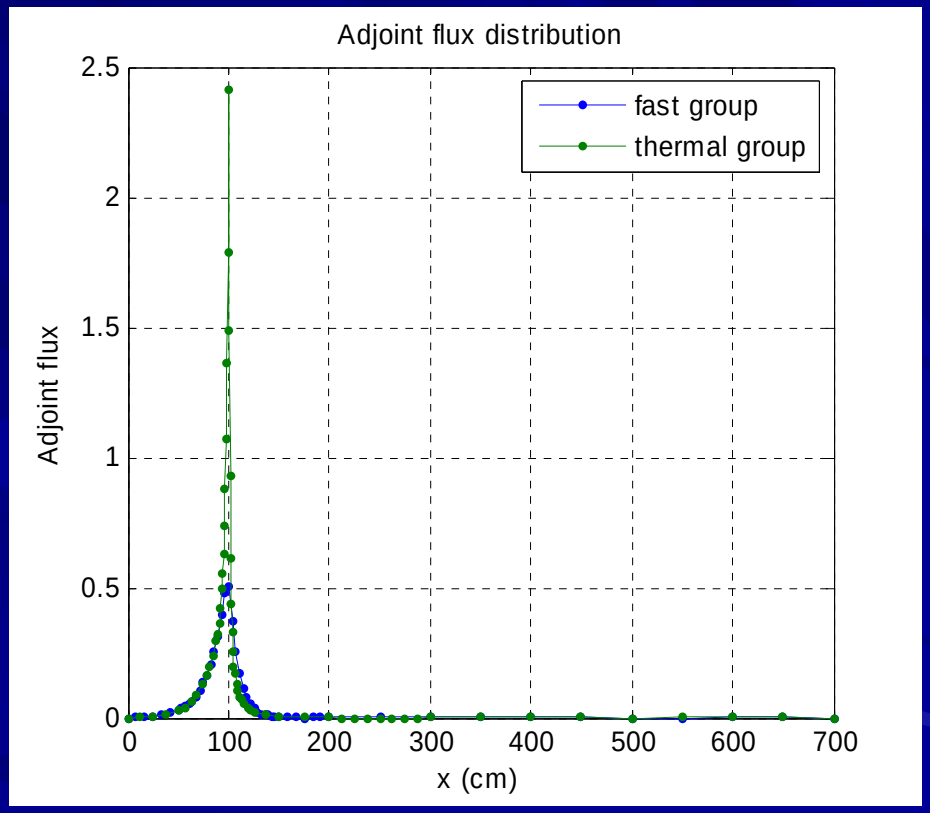
Goal-oriented hp-Adaptive Mesh Refinement: results

- GOAL: Point-wise flux at x= 100

Goal-oriented hp-solution, tol=1%



Goal-oriented adjoint flux



Mesh adaptation for Sn Transport

- Work in progress …

- Ideas:
  - To propose an additional flux solver option for NEWT (2D SN Transport)
  - Flux solver → DGFEM (Discontinuous Galerkin FEM)
  - As with all FEM techniques, properties of DG techniques have been intensively investigated by mathematicians, reliable error estimates exist; we'll apply DG mesh adaptivity techniques to transport (not as easy as it sounds…)

- So far,
  - Translated a NEWT geometrical description into a triangular mesh upon which DG will be applied

Mesh adaptation for Sn Transport

- NEWT mesh:

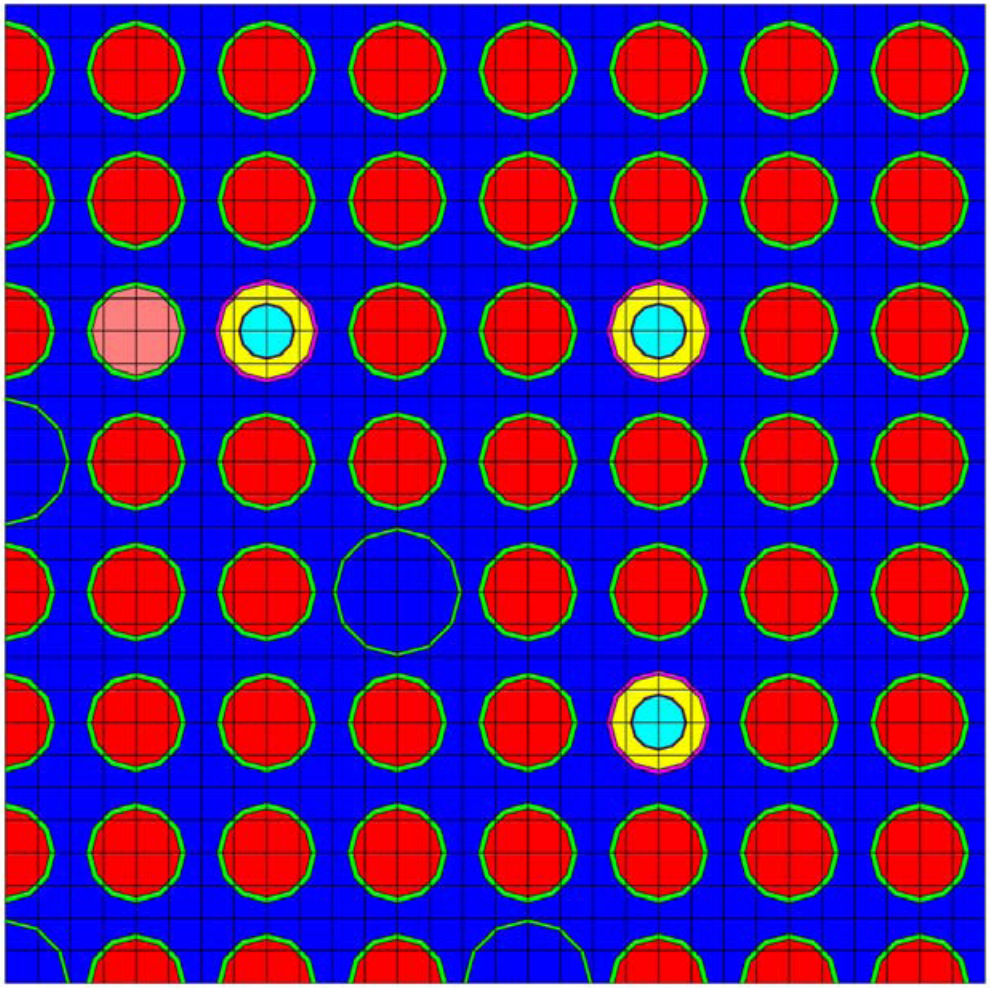
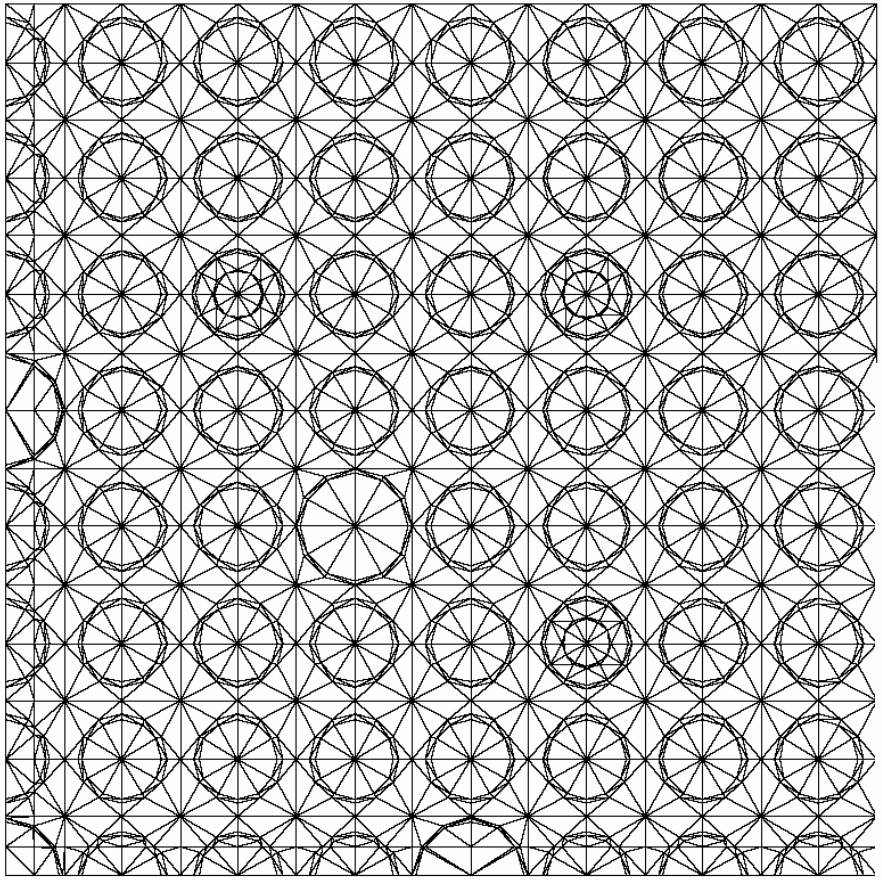
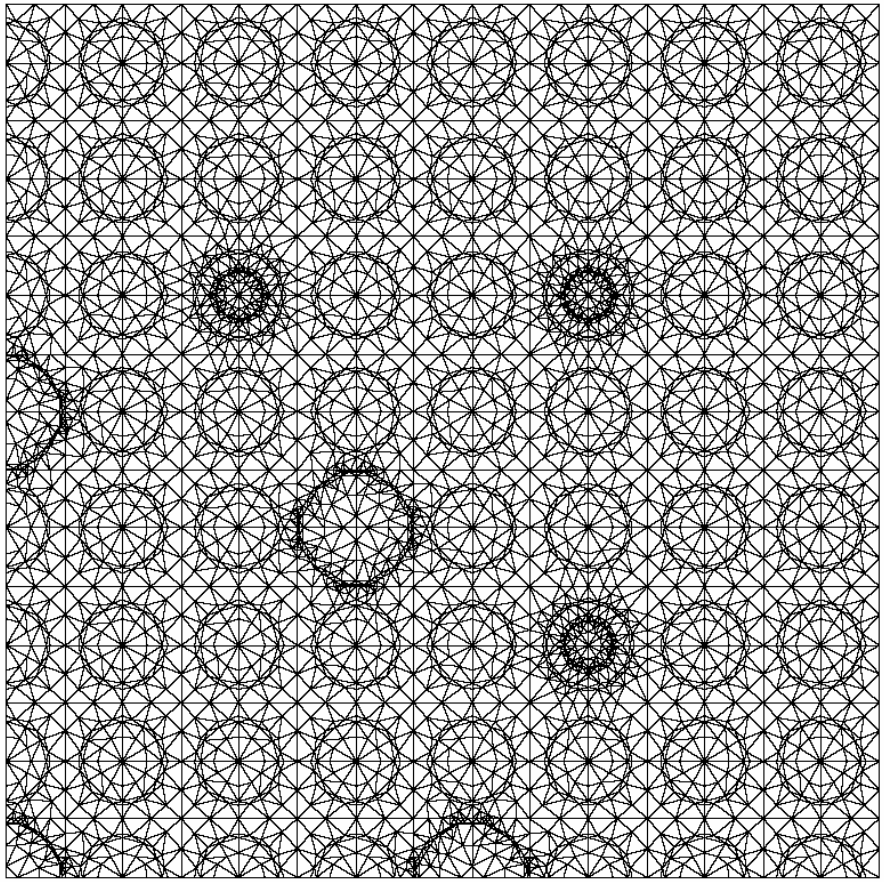


Figure F21.4.9. Mixture placement for quarter-assembly model of Example 4.

Mesh adaptation for Sn Transport





Conclusions

- Numerical error is intrinsic to the computer simulation of physical phenomena
- Sensible usage of available resource naturally favors **automatic mesh adaptivity**
- In the last decade or so, the theory of ***a posteriori* error estimations** has matured and allows the measure, control, and minimization of approximation errors.
  - In this theory, the computed solution itself is used to inexpensively provide point-wise error estimations.
  - By effectively estimating the error, the entire computational process can be seen as the **control of the error** in a succession, within a single calculation, of adaptively refined meshes.
  - → This should be one major component towards the goal of guaranteed-accuracy solutions (along with uncertainties assessment)
- More recently, goal-oriented computations have been combined with mesh adaptation to adapt the mesh only in regions of importance towards a certain **quantity of interest** (use of a dual or adjoint solution).

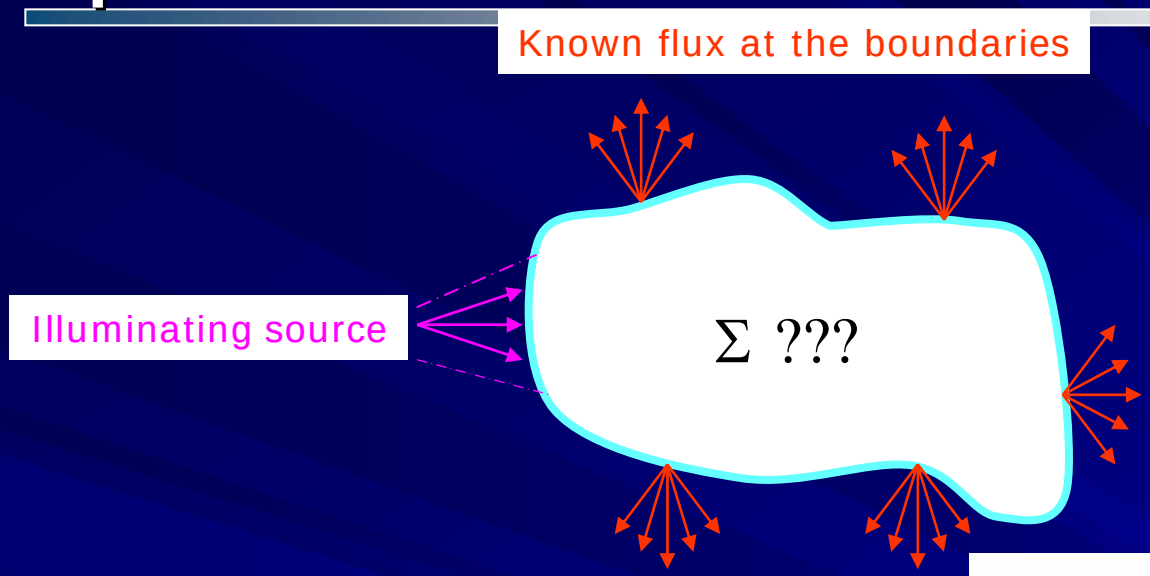
… and then some … Inverse problems

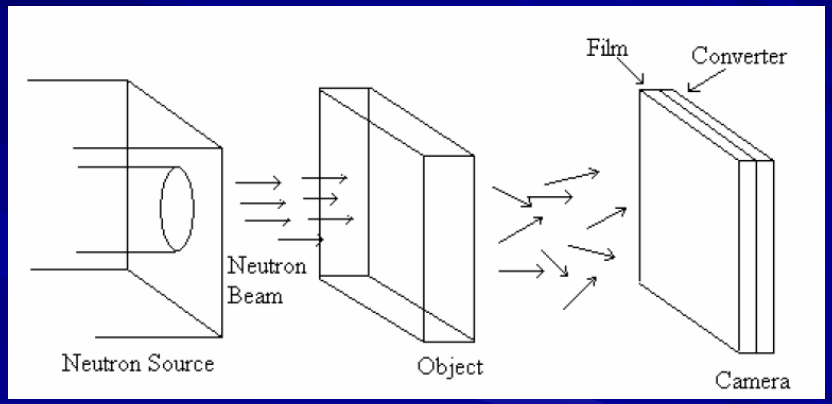
- What are inverse problems?

- Let first answer what are (usual) direct problem. In a direct problem,
  - the givens are:
    - The domain geometry
    - The material properties
    - The boundary conditions (e.g., inflow of particles)
  - The unknowns are:
    - The fluxes in the domain

- For an inverse problem,
  - the givens are:
    - The domain geometry
    - The fluxes in a part of the domain (could be known only at the boundary, e.g., outflow of particles)
    - The boundary conditions (e.g., inflow of particles)
  - The unknowns are:
    - The material properties

A pix



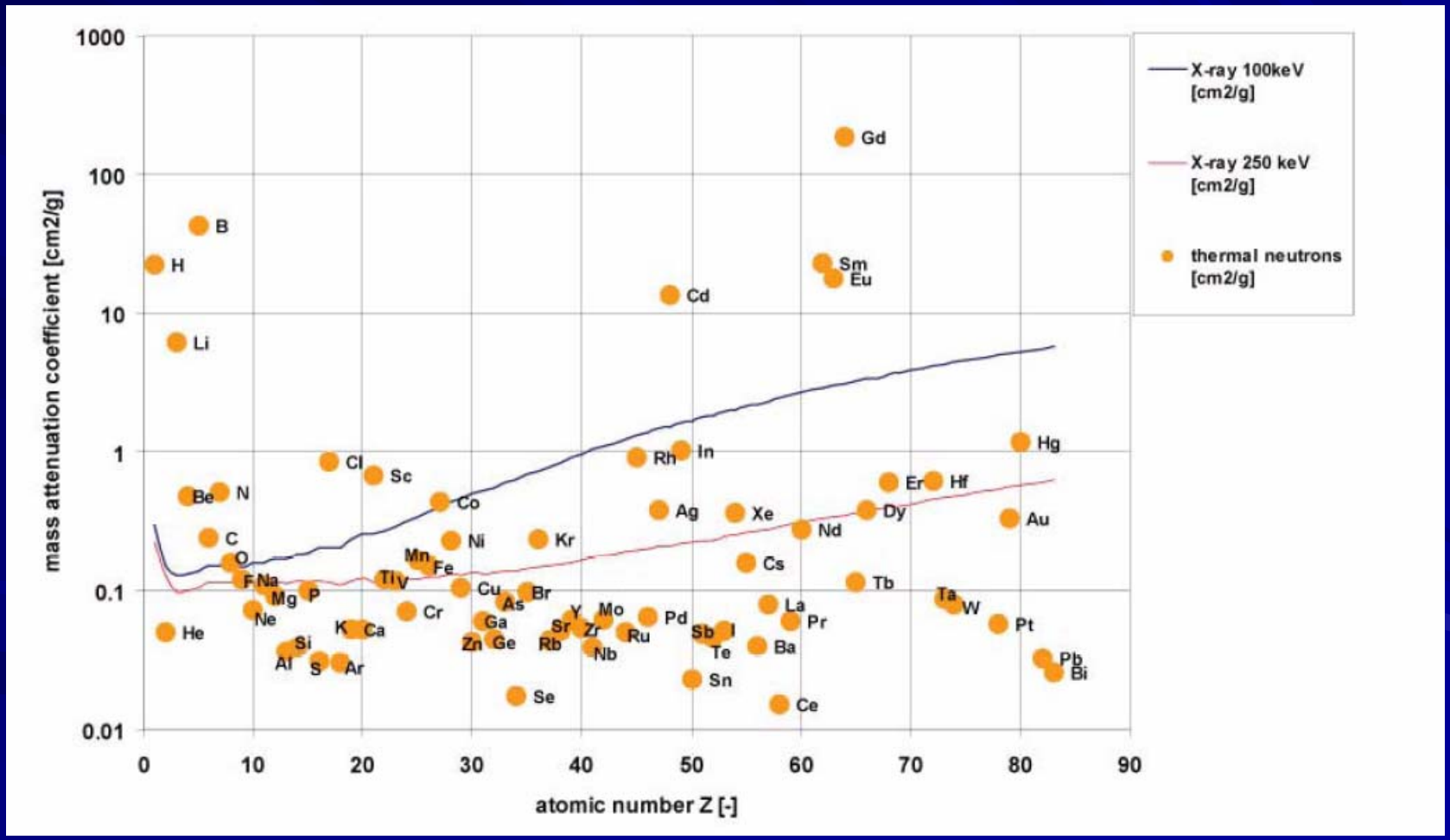


Applications:

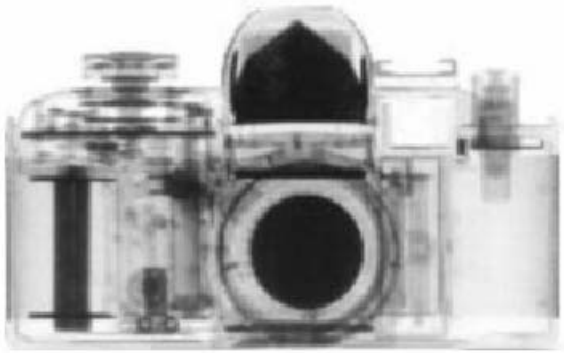
- Biomedical field (computed tomography X-ray scan, computed tomography MRI)
- Border control (detection of smuggled Special Nuclear Material)

X-ray vs. neutron CT

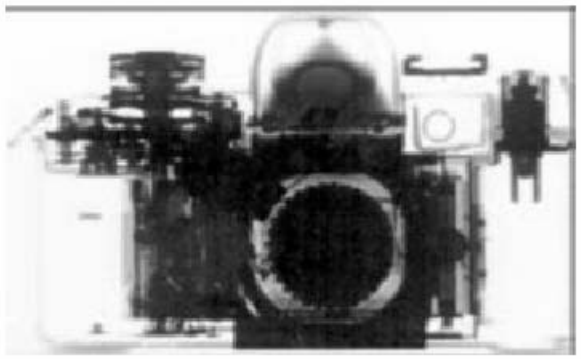
- Choice of incident particle is important:
  - X-rays cannot help in differentiating nuclei (same Z, but different A)
  - Deep penetration in high-Z material is troublesome for X-rays



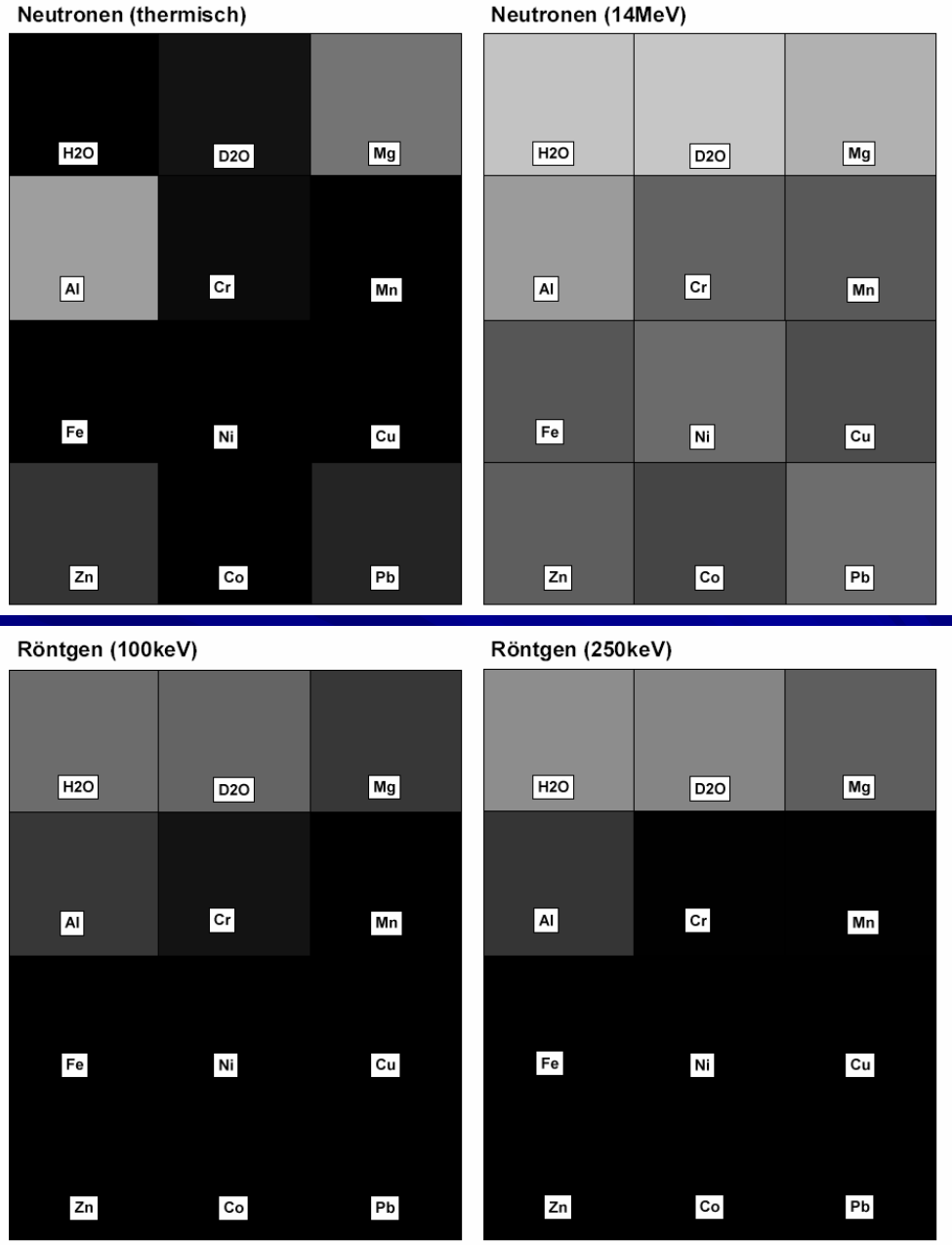
From http://neutra.web.psi.ch



Neutron radiography



X-ray radiography



Issues with current CT techniques

- Current reconstruction algorithms use in ‘inverse Radon transform’ to reconstruct the inside of an object.
- Main assumption in the procedure: scattering is ignored
- But scattering can decrease the resolution or worse

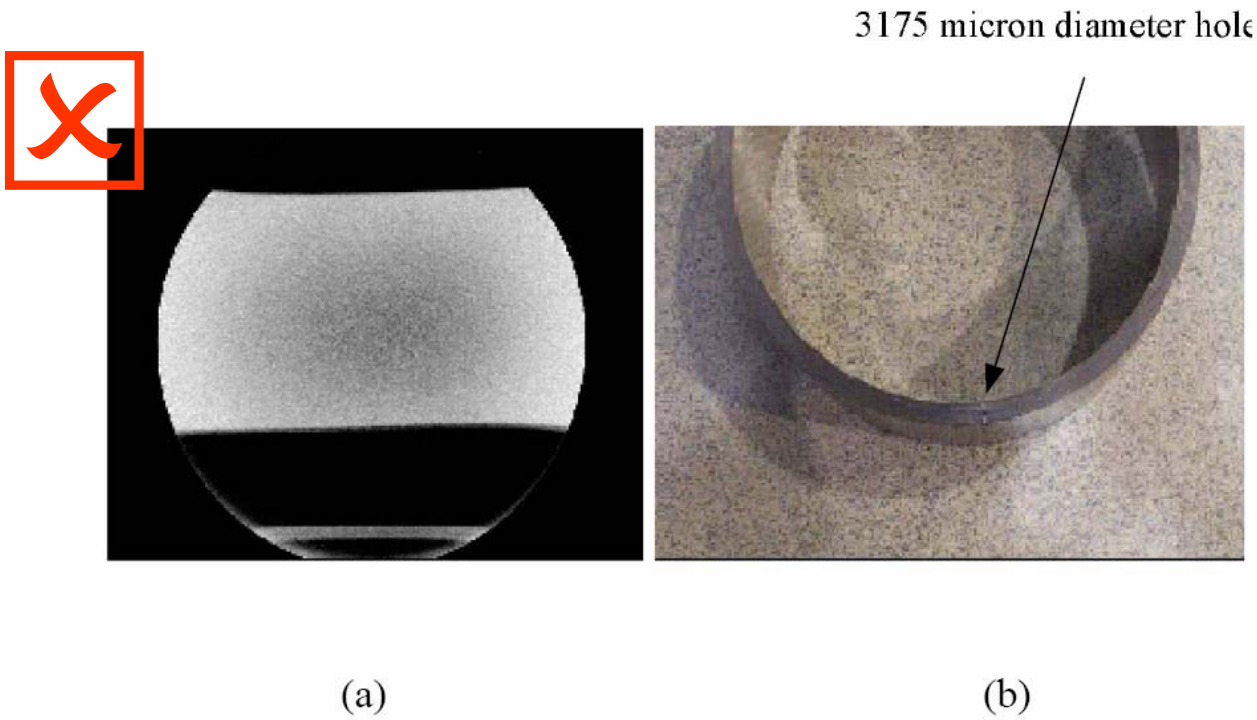


Fig. 4. Image on the left (a) is a neutron radiograph of a thick carbon fiber composite object with a 1/8th inch hole present. Image on the right (b) shows the object and the hole.

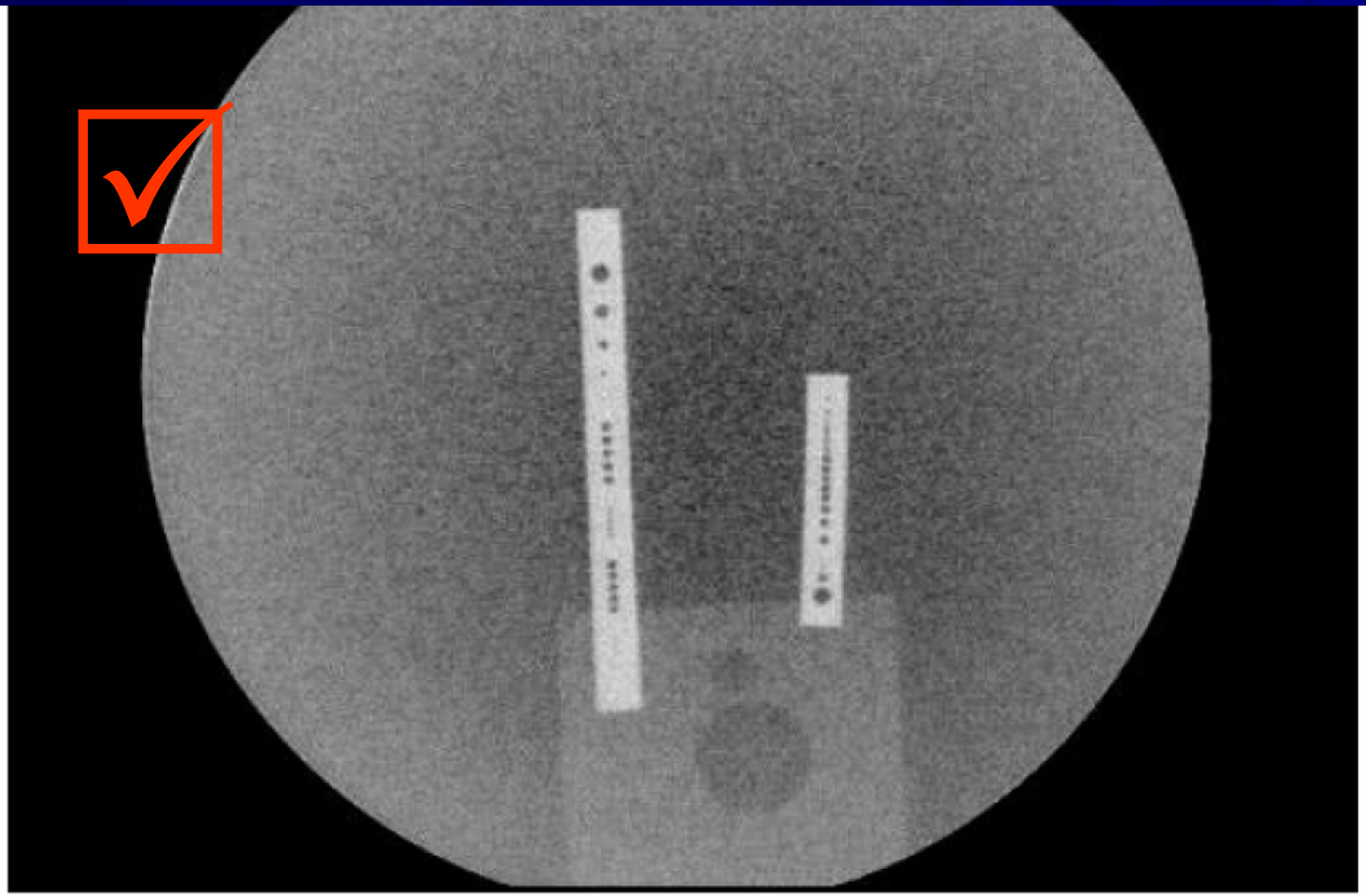


Fig. 3. Neutron radiograph of two cadmium strips displaying good image resolution for highly absorbing, low scattering materials. Each strip contains a number of different sized holes. The strips are supported on an aluminum plate.

Some scalar products and the duality principle

- Let the direct and adjoint transport problems be:

$$\left.\begin{aligned} B\Psi &= S, \quad in\ X \\ \Psi &= \Psi_{in}, \quad on\ \Gamma_- \end{aligned}\right\} \qquad \left.\begin{aligned} B^\dagger\Psi^\dagger &= S^\dagger, \quad in\ X \\ \Psi^\dagger &= \Psi^\dagger_{out}, \quad on\ \Gamma_+ \end{aligned}\right\}$$

$$\begin{aligned} X &= D \times \varepsilon \times (4\pi) \\ \Gamma_\pm &= \partial D \times \varepsilon \times (2\pi)_\pm \\ \Psi(x) &\quad x = (\mathbf{r}, E, \mathbf{\Omega}) \end{aligned}$$

where the transport operators are

$$B = \mathbf{\Omega}\cdot\nabla + \Sigma - H - P$$

$$B^\dagger = -\mathbf{\Omega}\cdot\nabla + \Sigma - H^\dagger - P^\dagger$$

- Defining the following scalar products:

$$(f,g) = \int_D d\mathbf{r} \int dE \int_{(4\pi)} d\mathbf{\Omega}(fg)(\mathbf{r},E,\mathbf{\Omega})$$

$$< f,g >_\pm = \int_\Gamma dS \int dE \int_{(2\pi\pm)} d\mathbf{\Omega} \left|\mathbf{n}\cdot\mathbf{\Omega}\right| (fg)(\mathbf{r},E,\mathbf{\Omega})$$

- Duality is a generalized conservation statement

$$(\Psi^\dagger, S) + < \Psi^\dagger, \Psi_{in} >_- = (S^\dagger, \Psi) + < \Psi^\dagger_{out}, \Psi >_+$$

Functional to be minimized

- The functional to be minimized is a measure of the discrepancy at the boundary Γ of the domain between
  - the neutron fluxes Ψ obtained by solving the transport equation and
  - the measured fluxes Ψ^{REF}.

- Regularization terms, β, can be added to suppress unwanted features in the parameters Σ. The type of regularization is usually dictated by the application and insight into physical and unphysical features of solutions (here, we want $0<\Sigma<\infty$).

- Constrained minimization case:

$$F(\Psi,\Sigma)=\frac{1}{2}\left\langle \Psi-\Psi^{REF},\Psi-\Psi^{REF}\right\rangle_{+}+\beta(\Sigma)$$

Nonlinear optimization process

- The reconstruction problem is a nonlinear optimization problem.
  - Find the distribution of the optical properties Σ of the object under scrutiny so that :

the neutron fluxes Ψ recovered at the boundary Γ of the domain best match the measured data Ψ^{REF}.

i.e., *F* is minimized.

First sketch of the optimization algorithm:

1. material properties Σ^{ℓ} are given,
2. Solve for Ψ
3. Evaluate *F*
4. IF *F* > tolerance

   Compute a new set of material properties $\Sigma^{\ell+1}$ and go back to step 2

   ELSE

   Problem has converged

   ENDIF

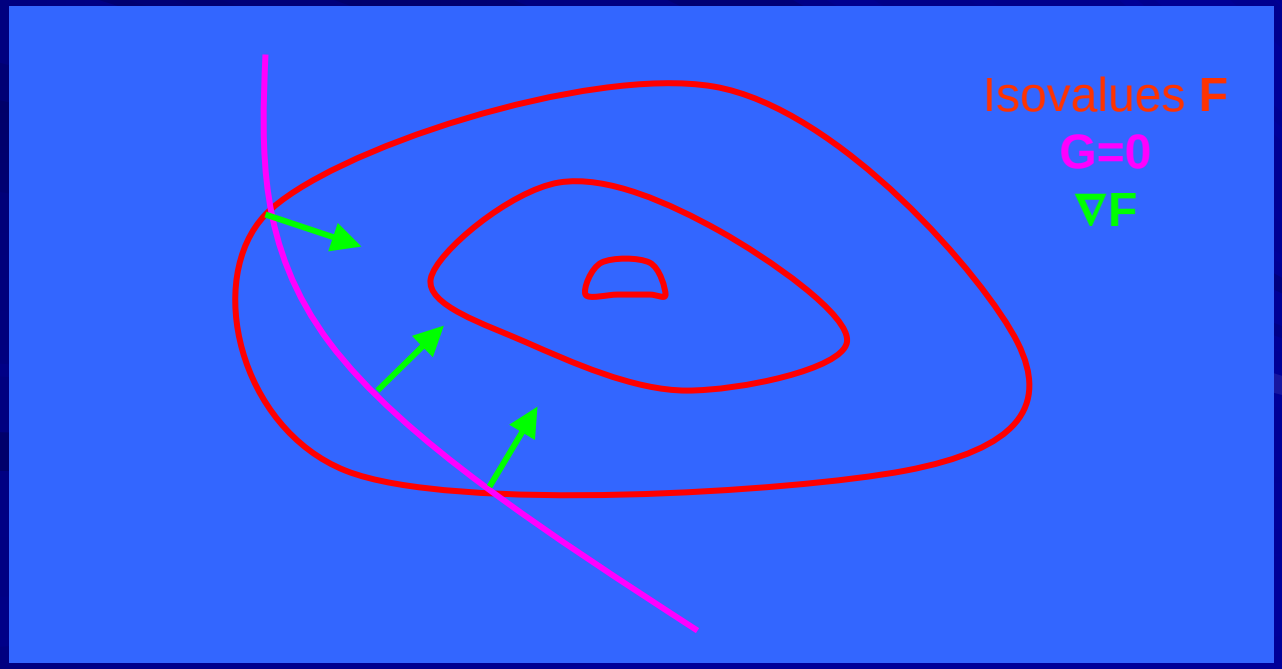
Optimization 101

- Unconstrained case:

$$\text{If } F(x) \in C^1, \quad \text{then } \min_x F \Leftrightarrow \nabla F = 0.$$

- Constrained case:

$$\text{Find } \min_x F \quad \text{such that } G(x) = 0 \Leftrightarrow \begin{cases} \nabla F \propto \nabla G \\ G(x) = 0 \end{cases} \Leftrightarrow \begin{cases} \nabla F + \lambda \nabla G = 0 \\ G(x) = 0 \end{cases}$$



- Introducing the function (Lagrangian $\mathcal{L}$) $\boxed{L = F + \lambda G}$

$$\text{Find } \min_x F \quad \text{such that } G(x) = 0 \Leftrightarrow \begin{cases} \nabla F + \lambda \nabla G = 0 \\ G(x) = 0 \end{cases}$$

$$\Leftrightarrow \begin{cases} \dfrac{\partial L}{\partial x} = \nabla F + \lambda \nabla G = 0 \\ \dfrac{\partial L}{\partial \lambda} = G(x) = 0 \end{cases}$$

- The PDE-constrained problem involves the Lagrangian functional $\mathcal{L}$:

$$\mathcal{L}(\Psi,\Sigma,\Psi^{\dagger}) = \frac{1}{2}\left\langle \Psi - \Psi^{REF}, \Psi - \Psi^{REF} \right\rangle_{+} + \left(\Psi^{\dagger}, B\Psi - S\right) + \left\langle \Psi^{\dagger}, \Psi - \Psi^{inc} \right\rangle_{-}$$

- The optimality conditions are given by the stationary of the Lagrangian $\mathcal{L}$, i.e.,

$$\partial_x \mathcal{L}(\Psi,\Sigma,\Psi^{\dagger}) = 0 \quad \text{for } x = \{\Psi,\Sigma,\Psi^{\dagger}\}$$

$$(1) \quad \frac{\partial \mathcal{L}}{\partial \Psi} = \left(1, B^{\dagger}\Psi^{\dagger}\right) + \left\langle 1, \Psi^{\dagger} - \Psi + \Psi^{REF} \right\rangle_{+}$$

$$(2) \quad \frac{\partial \mathcal{L}}{\partial \Sigma} = \left(\Psi^{\dagger}, (\partial_{\Sigma} B)\Psi\right)$$

$$(3) \quad \frac{\partial \mathcal{L}}{\partial \Psi^{\dagger}} = \left(1, B\Psi - S\right) + \left\langle 1, \Psi - \Psi^{inc} \right\rangle_{-}$$

  - Eq 1: adjoint problem [adjoint flux = Lagrange multiplier in optimization] driven by the misfit outgoing source at the boundary
  - Eq 3: forward problem [the 'constraint']
  - Eq 2: minimum w.r.t. to material properties

$$\Sigma^{\ell+1} = \Sigma^{\ell} - \alpha_{\ell}\left(\Psi^{\dagger}, (\partial_{\Sigma} B)\Psi\right)$$

- Goal : stationarity of the Lagrangian

$$\boxed{\partial_x \mathcal{L}(\Psi, \Sigma, \lambda) = 0 \quad \text{for } x = \{\Psi, \Sigma, \lambda\}}$$

- Use a Newton's method to solve that problem:

$$\boxed{\begin{cases} \partial_{xx} \mathcal{L}(x^\ell) \delta x^{\ell+1} = -\partial_x \mathcal{L}(x^\ell) \\ x^{\ell+1} = \delta x^{\ell+1} + x^\ell \end{cases}}$$

- The Hessian of the Lagrangian is needed but many second derivatives terms vanish because the transport operator is linear in both Σ and Ψ.

Previous work (Dr. Bangerth b/c he has ***prettier*** pix)

- **Fluorescence enhanced optical tomography** is a relatively new medical imaging modality:

- A pulsed laser illuminates the skin, and light diffuses into the tissue
- Light is absorbed by a dye that is previously injected and accumulates in tumors
- The dye emits fluorescent light that diffuses throughout the tissue
- Fluorescent light amplitude and phase is recorded on the skin

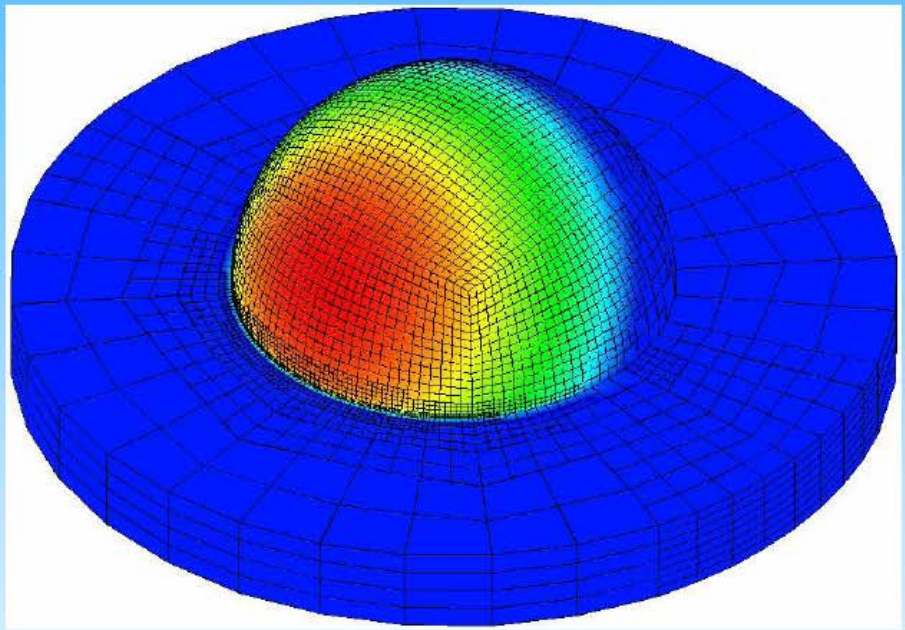
- Inverse problem:
  - Try to reconstruct dye concentrations from the measured fluorescent light
  - Hard problem since the setting is inherently 3-D, rather high resolution is required, and the problem is very ill-posed due to the diffusive process

Optical tomography examples

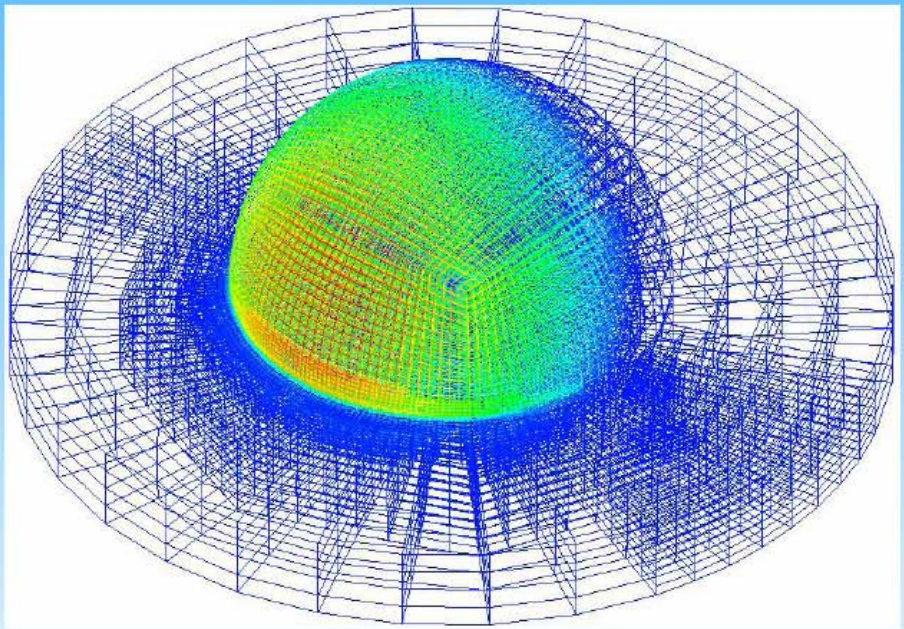
Adaptive meshes for breast phantom geometry (B., Joshi, Sevick, 2005):

- Hemisphere of 5cm radius on disk of 10cm radius and 2cm height
- Target has 1cm diameter and is 1.5cm under the surface

- Forward mesh has 34,000 cells (a uniform one would have 9.4M)



Surface of mesh used for forward modeling



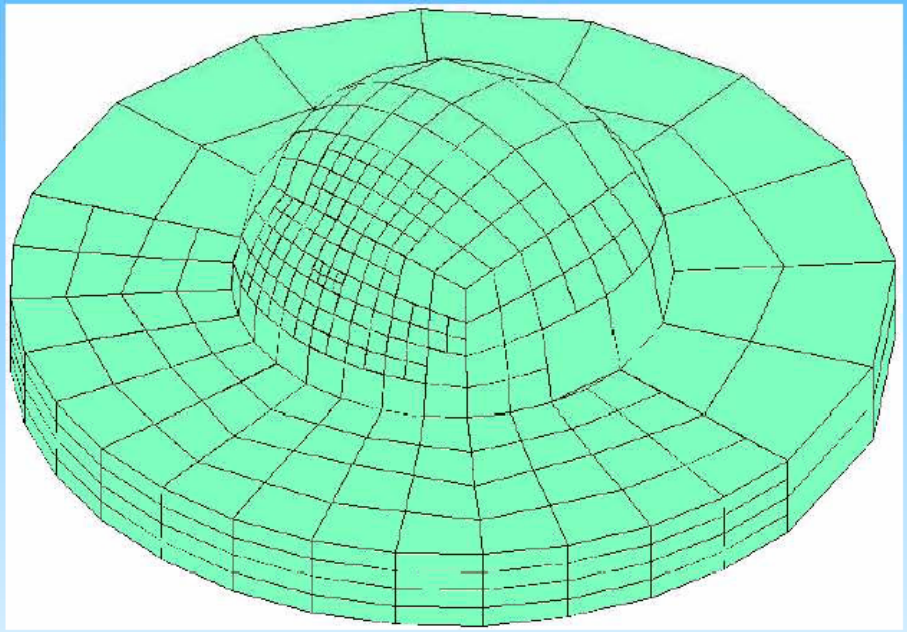
Interior of mesh used for forward modeling

Optical tomography examples

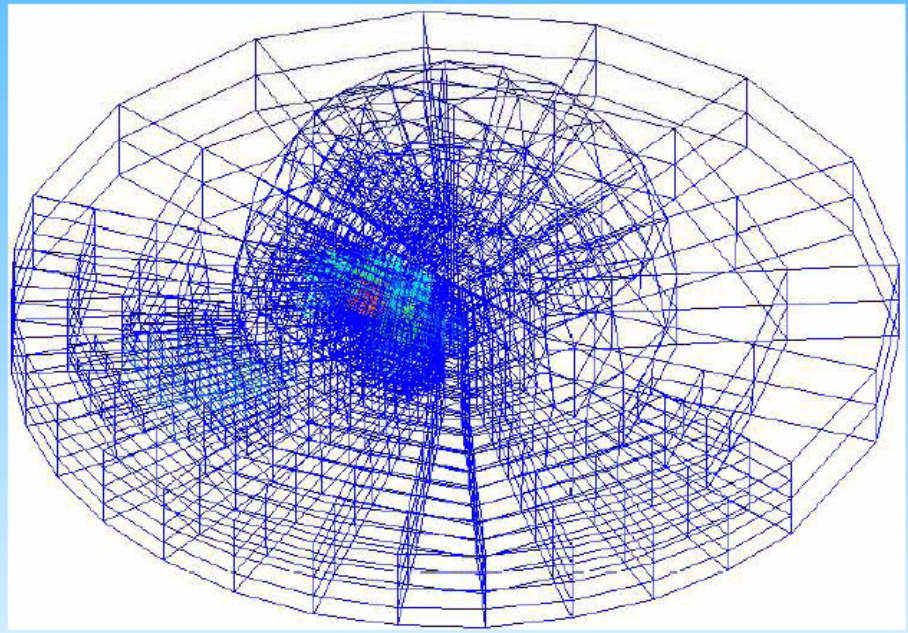
Adaptive meshes for breast phantom geometry (B., Joshi, Sevick, 2005):

- Hemisphere of 5cm radius on disk of 10cm radius and 2cm height
- Target has 1cm diameter and is 1.5cm under the surface

- Reconstruction mesh has 2500 cells (a uniform one would have 1.2M)



Surface of mesh used for reconstruction

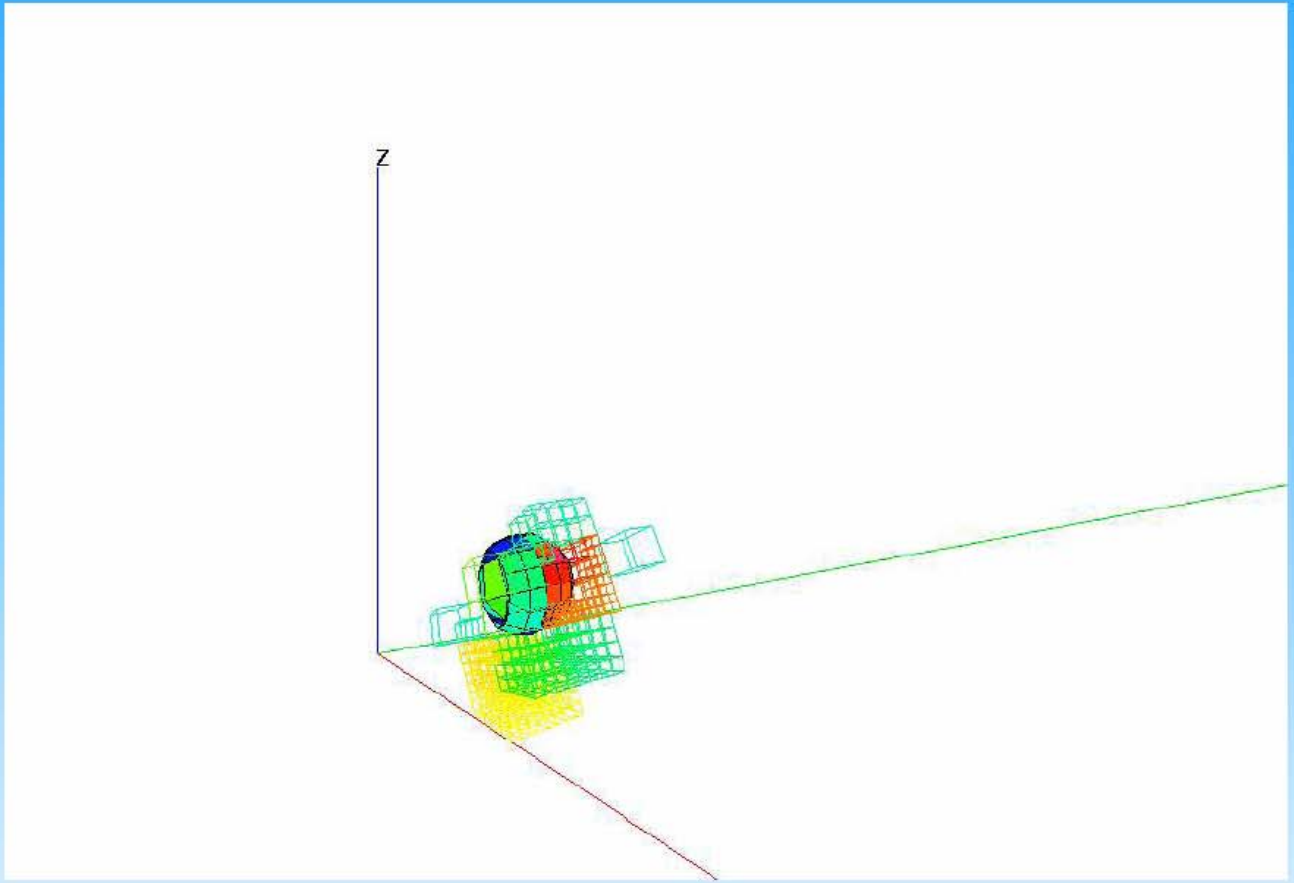


Interior of mesh used for reconstruction

Optical tomography examples

Reconstruction for breast phantom geometry (B., Joshi, Sevick, 2005):

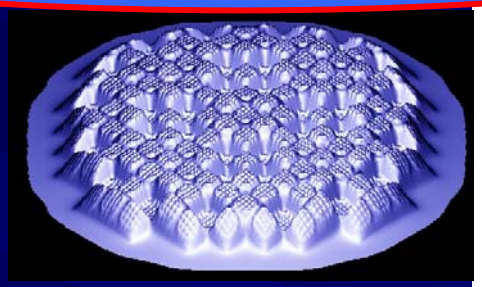
Cells with highest dye concentration (wireframe) and exact target location and size (sphere)

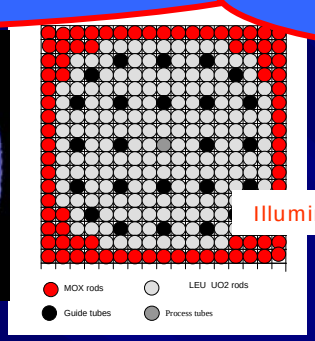


Adaptive resolution around the target: 0.625 mm in a target volume of 890 cm^3.

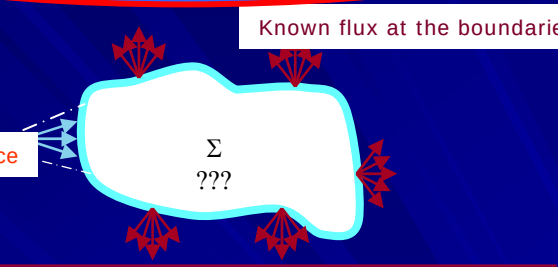
Summary

Reactor core and assembly designs



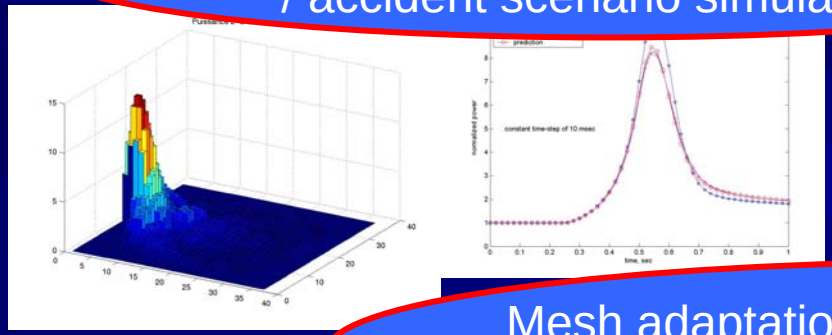


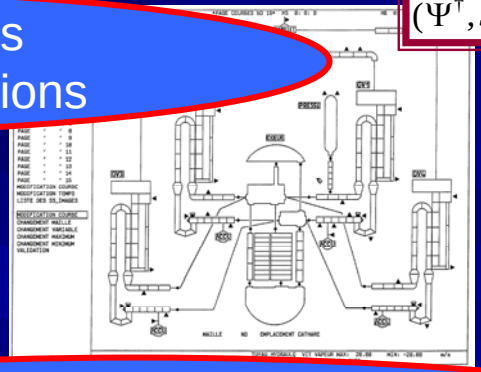
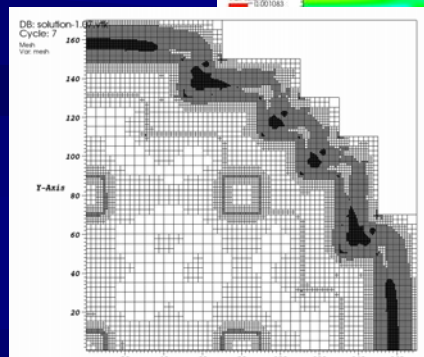
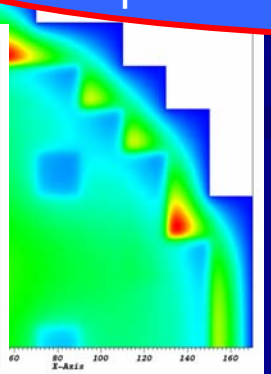
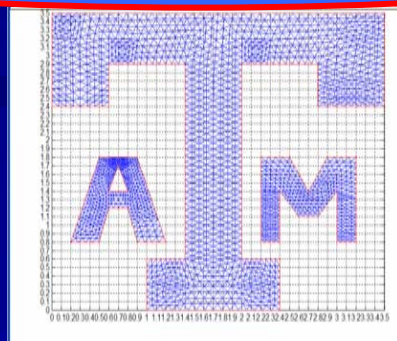
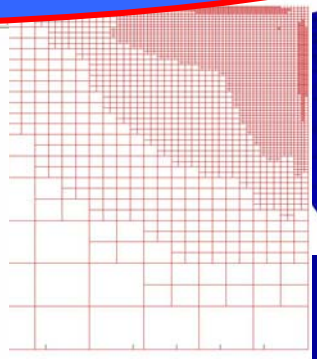
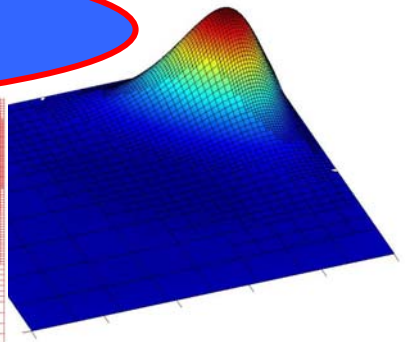
Smuggled Material Detection Methodology



$$(\Psi^{\dagger}, S) + < \Psi^{\dagger}, \Psi_{in} >_{-} = (S^{\dagger}, \Psi) + < \Psi^{\dagger}_{out}, \Psi >_{+}$$

High fidelity multi-physics / accident scenario simulations





Mesh adaptation for solving neutron balance equations accurately on complex geometries