

hp—AMR applied to the neutron transport equation discretized by a Discontinuous Galerkin upwind scheme

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- Nuclear reactor core physics (see F. Madiot's presentation)
- For "Sodium Fast Reactors" (SFR), the diffusion (or SP_N) approximation is deemed insufficient for core design calculations (homogenized assemblies)
- In the early stage (2009-2012) of the ASTRID prototype (cancelled in 2019) design studies, development of a 3D neutron transport solver to supplement the existing ERANOS code

SNATCH solver

Along the following lines:

angular discretization: so-called S_N method (quadrature-based):

$$\vec{\Omega} \in S_2 \to \left(w_n, \vec{\Omega}_n\right)_{1 \le n \le N}$$

- high-order spatial scheme → Discontinuous Galerkin (DG) upwind scheme
- both direct and adjoint solutions → perturbation theory toolbox

With the additional idea of having a modular environment to test numerical methods

▶ In this framework, AMR has been investigated

This presentation

the salient features of this (old) work + "links" to more recent works by other researchers on this subject

Cea Contents

- Equations system and spatial discretization
 - Semi-discrete equations system
 - Spatial discretization
- hp-Adaptive Mesh Refinement
- *hp* AMR principle and "ingredients"
- Error evaluation for AMR

Application to SFR reactor cores

- Benchmarks description and h–AMR results
- Comparison of various hp-AMR strategies
- Energy group dependent h—AMR

AMR and Perturbation theory

- Extension of the standard perturbation formula to spatial discretization effects
- Possible uses in the AMR framework

Summary and perspectives

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Cea Semi-discrete equations system

A spatial domain \mathcal{D} and its boundary Γ with $\forall \vec{\Omega} \in S_2$, $\Gamma = \Gamma_{-}(\vec{\Omega}) \dot{\cup} \Gamma_{+}(\vec{\Omega})$

Pseudo-stationary neutron transport equation + Multigroup (energy) and S_N (angle) discretizations Semi-discrete matrix form

$$\underline{\underline{H}}\underline{\phi}(\vec{r}) - \underbrace{\underline{\underline{s}}\underline{\phi}(\vec{r}) - \frac{1}{k}\underline{\underline{F}}\underline{\phi}(\vec{r})}_{\underline{\underline{s}}(\vec{r})} = 0 \quad \text{where} \quad \underline{\phi} = \left[\phi_n^g(\vec{r}) = \phi^g(\vec{r}, \vec{\Omega}_n)\right]_{(g,n)}$$

with

$$\begin{split} \underline{H} &= \operatorname{diag} \left[\vec{\Omega}_{n} \cdot \vec{\nabla} + \bar{\Sigma}_{t}^{g}(\vec{r}) \right]_{(g,n)} \\ \underline{S} &= \left[\frac{w_{n'}}{4\pi} \sum_{l=0}^{L} (2l+1) \sum_{m=-l}^{l} \mathcal{R}_{l,m}(\vec{\Omega}_{n}) \bar{\Sigma}_{s,l}^{g \leftarrow g'}(\vec{r}) \mathcal{R}_{l,m}(\vec{\Omega}_{n'}) \right]_{(g,n),(g',n')} \\ \underline{F} &= \left[\frac{w_{n'}}{4\pi} \chi^{g}(\vec{r}) \nu \Sigma_{f}^{g'}(\vec{r}) \right]_{(g,n),(g',n')} \end{split}$$

- a *dominant eigenvalue problem* with e.g. "void" boundary condition: $\forall g, \forall n, \forall \vec{r} \in \Gamma_{-}(\vec{\Omega}_{n}), \phi_{n}^{g}(\vec{r}) = 0$
- ▶ *Iterative approach* to solve the *source-flux dependency*: classically, three nested iterative loops: e.g. power method (fission) \supset Gauss-Seidel ($g \leftarrow g'$ scattering) \supset Richardson ($g \leftarrow g$ scattering)

Cea Spatial discretization

- Mesh $M_h = \{\kappa\}$ (structured mesh of lozenges) with cell-wise constant cross-sections
- ▶ Discontinuous Galerkin upwind scheme [Reed and Hill, 1973] with non uniform order $(\mathcal{M}_{p}^{h} = \{(\kappa, p_{\kappa})\}_{\kappa \in \mathcal{M}_{p}})$

For any group and direction (g, n indices omitted), the approximation of ϕ is considered as

$$\phi_h \in V_h^{\mathbf{p}} = \left\{ \mathbf{v} \in L^2(\mathcal{D}) : \forall (\kappa, p_\kappa) \in \mathcal{M}_h^{\mathbf{p}}, \mathbf{v}|_\kappa \in Q_{p_\kappa}(\kappa) \right\}$$

On any κ , it obeys the following *local weak form*: $\forall \varphi_h \in V_h^{\mathbf{p}}$,

$$\left\langle \varphi_{h}, \left(\vec{\Omega} \cdot \vec{\nabla}_{h} + \Sigma_{t,\kappa}\right) \phi_{h} \right\rangle_{\kappa} + \left\langle \varphi_{h}^{+}, \left[\!\left[\phi_{h}\right]\!\right] \right\rangle_{\partial \kappa_{-}} = \left\langle \varphi_{h}, S \right\rangle_{\kappa}$$

where

$$\begin{aligned} &- \partial \kappa_{\pm} = \left\{ \vec{r} \in \partial \kappa : \vec{\Omega} \cdot \vec{n}(\vec{r}) \ge 0 \right\} \\ &- \phi_h |_{\partial \kappa}^{\pm}(\vec{r} \in \partial \kappa) = \lim_{s \to 0^{\pm}} \phi_h\left(\vec{r} + s\vec{\Omega}\right) \\ &- \left\langle f, g \right\rangle_{\partial \kappa_-} = \int_{\partial \kappa_-} d^2 r \left| \vec{\Omega} \cdot \vec{n}(\vec{r}) \right| fg \\ &- \left[\left[\phi_h \right] \right] = \left(\phi_h^+ - \phi_h^- \right) \end{aligned}$$

- special case of stabilization by *jump penalization* [Brezzi et al., 2004, Brezzi et al., 2006]
- very well suited in this context:
 - direction-dependent cell-by-cell sweeping
 - cell-wise linear system inversion

Cea Spatial discretization

- ► Hierarchical polynomial basis $\Xi_p(\hat{\kappa}) = \{f_i\}_{i \in [1, \dim(Q_p(\hat{\kappa}))]}$ s.t. $\Xi_p(\hat{\kappa}) \subset \Xi_{p+1}(\hat{\kappa}), \forall p \in \mathbb{N}$
- Adapted from [Shephard et al., 1997], $\Xi_p(\hat{\kappa})$ is based on
 - the topological hierarchy of mesh entities (vertices, edges, faces and cells) that define the closure of \hat{k} of $\hat{\kappa}$

$$\bar{\hat{\kappa}} = \left\{ M_{\hat{\kappa}}^d, \partial M_{\hat{\kappa}}^d \right\} = \left\{ M_{\hat{\kappa}}^d, M_{\hat{\kappa}}^d \{ M_{\hat{\kappa},j'}^1 \}, \dots, M_{\hat{\kappa}}^d \{ M_{\hat{\kappa},j'}^0 \} \right\}$$

where $M_{\hat{\kappa}}^d \{M_{\hat{\kappa},j'}^{d'}\}$ is the $(j')^{\text{th}}$ entity of dimension d' bounding the reference element $\hat{\kappa}$

- with basis functions obtained by associating shape functions to these entities s.t. any basis function associated with $M_{c}^{d'}$, vanishes over all "lower order" bounding entities except $M_{c}^{d'}$,

 \rightarrow of particular interest while propagating the flux from one element to the other through the boundary trace



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hp- AMR principle and "ingredients"

General objective: improve in an "optimal" way (vs. number of discretisation dofs, cpu time) the
approximate solution accurary



 Back in 2008, little interest in neutronics : S_n – DG – 2D triangular meshes [Ragusa and Wang, 2010, Wang and Ragusa, 2011]

Damien Fournier's Ph.D. thesis (2008-2011)

directed by Raphaèle Herbin from the "Institut de Mathématiques de Marseille"

Error evaluation for AMR: general ideas

- Quantity of interest: the *error on the flux* e.g. $\|e\|_{L^2(\kappa)} = \|\phi_h \phi\|_{L^2(\kappa)}$ (vs. "goal-oriented" method)
- Local refinement process: "efficient" evaluation of the *cell-wise error* associated with ϕ_h
 - analysis of an *a posteriori estimator under "minimal" regularity hypotheses* ($\phi \in W^{1,1} \cap L^{\infty}$)
 - "simplifications" in order to get an "efficient" error indicator E^{FV}
- ▶ "Optimal" choice between *h*− or *p*−*refinement*:
 - to be naturally related to the "local" regularity of $\phi \dots$
 - regularity s of $\phi \ (\in H^s)$ limited to $\frac{1}{2} \varepsilon$ or $\frac{3}{2} \varepsilon$
 - loss of regularity in the neighbourhood of characteristic lines directed along $\vec{\Omega}_n$



- \rightarrow analysis of an *a posteriori* estimator under strong regularity hypotheses ($\phi \in C^{\infty}$): combined with E^{FV} , E^{R} as a "local" regularity indicator
 - ... but also to the convergence regime in p (pre-asymptotic vs. asymptotic) about which a priori error estimation (global) results can give useful information
- ightarrow accordingly, different hp- strategies have been constructed and compared

Cea Error evaluation for AMR: *a priori* error estimation

► Global error convergence vs. uniform refinement (order p, normalized mesh size h)

$$\|e\|_{L^{2}(\mathcal{D})} = \epsilon_{p,h} = \mathcal{O}\left(\frac{h^{\min(p+1,s)}}{p^{\alpha}}\right)$$

with $s = \frac{1}{2} - \varepsilon$ (MMS0) or $s = \frac{3}{2} - \varepsilon$ (MMS1) (theoretical results e.g. [Houston and Süli, 2001] + numerical tests using manufactured solutions)



Error evaluation for AMR: *a priori* error estimation

Global error convergence vs. uniform refinement (order p, normalized mesh size h)

$$\|e\|_{L^{2}(\mathcal{D})} = \epsilon_{p,h} = \mathcal{O}\left(\frac{h^{\min(p+1,s)}}{p^{\alpha}}\right) \text{ avec } \alpha = \begin{cases} s - \frac{1}{2} & \text{asymptotic} \\ s & \text{pre-asymptotic} \end{cases}$$

with $s = \frac{1}{2} - \varepsilon$ (MMS0) or $s = \frac{3}{2} - \varepsilon$ (MMS1)
(theoretical results e.g. [Houston and Süli, 2001] + numerical tests using manufactured solutions)

► Refinement "performance" evaluated through $J_{p \to p', h \to h'} = \frac{\left|\log(\epsilon_{p', h'}) - \log(\epsilon_{p, h})\right|}{\log(dof_{p', h'}) - \log(dof_{p, h})}$ (dof_{p, h}, number of degrees of freedom)

• Comparison between
$$J_{p \to p+1,h}$$
 and $J_{p,h \to h/2}$: $\left(p - \text{refinement is "better" if } \frac{\alpha}{s} \ge \frac{\log\left(\frac{p+2}{p+1}\right)}{\log\left(\frac{p+1}{p}\right)}\right)$

A first important observation to be taken into account in an *hp*-strategy

- in the *pre-asymptotic regime* (resp. asymptotic), *p*-*refinement* (resp. *h*-refinement)
- numerical tests on MMS0 and MMS1: *pre-asymptotic regime, at least up to* p = 4

h

MMS1 (c $-\frac{3}{2}$)

2 log(p)

Cea Error evaluation for AMR: *a posteriori* estimators/indicators

Two estimators/indicators under very different regularity hypotheses

 E^R for $\phi \in C^{\infty}$ (strong regularity) [Fournier et al., 2011]



Cea Error evaluation for AMR: *a posteriori* estimators/indicators

Two estimators/indicators under very different regularity hypotheses

 E^{FV} for $\phi \in W^{1,1} \cap L^{\infty}$ (*"minimal" regularity*) [Fournier et al., 2013]

- rigorous a posteriori estimation based on [Dedner et al., 2007]
- "simplifications" \rightarrow error indicator: $E^{FV} = \sum_{b \in \mathcal{B}_h(\kappa)} S_b \int_b d^2 r \left| \vec{\Omega} \cdot \vec{n} \right| \left[\phi_h \right]$

 \rightarrow a "justification" of the heuristic use of such $[\![\phi_h]\!]$ -based indicators elsewhere e.g. [Owens et al., 2017]



Refined mesh with E^{FV} - MMS0



Error convergence – refinement driven by E^{FV} or E^{R} – MMS0

Cea Error evaluation for AMR: *a posteriori* estimators/indicators

- Two estimators/indicators under very different regularity hypotheses
- Two "supplementary" error estimators/indicators
- *E^R* : a "bad" estimator in our framework but an *indicator of the local regularity*
- E^{FV} : a "good" error indicator for the cells selection at each step of the AMR process

Error evaluation for AMR for neutronics equations system

- In all cases, a same spatial mesh for all directions $\vec{\Omega}_n$
 - cell-wise error indicator on the so-called scalar flux (angular flux integrated over S_2) $\bar{E}^{g}(\kappa) = \sum w_{n} E_{n}^{g}(\kappa)$
 - the source is "weakly" anisotropic \rightarrow mainly dependent on the scalar flux
- Two different approaches for the *energy groups*:
 - either, a same spatial mesh for all energy groups g



• refinement criterion: $\begin{pmatrix} \text{cell } \kappa^* \text{ of the spatial mesh of macro-group } \mathfrak{g} \text{ is refined iff} \\ \hat{E}^{\mathfrak{g}}(\kappa^*) \geq \alpha \max_{\kappa \in \mathcal{M}_h} \hat{E}(\kappa) \end{pmatrix}$ with α , a user parameter

- L_2 -projection operators for the construction of the group coupling source terms
- AMR loop "on top" of the power iteration loop for the eigenvalue problem solution

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Cea Benchmarks description and *h*-AMR results

- 2D and 3D benchmarks constructed from the ZONA2B core of the CIRANO experimental program (MASURCA, CEA Cadarache)
- steel reflector around the core: important flux variations at the interface with a very strong coupling between the space and energy variations
- core composed of three homogeneized and "condensed" (G = 33 energy groups) materials
 - FUEL (sodium + U/PuO₂ fuel)
 - REFLECTOR (3/4 steel + 1/4 sodium)
 - SHIELD (steel)
- initial non-conforming mesh coarsening in order to describe the geometry with a reduced number of cells



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In the frame of P. Archier's Ph.D. thesis, h - AMRAdaptive vs. uniform h-refinement for p = 2 (a same spatial mesh for all groups)

- flux error
$$\varepsilon_{L^2} = \max_g \sum_n w_n \|e_n^g\|_{L^2(\mathcal{D})}$$

w.r.t to a reference solution with a very fine mesh
and high order p

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- in 2D: flux error of 10^{-3}
 - \rightarrow computational time $\times 1/4$

→ in 3D: computational time of 5000s → *flux error* ×1/4

Cea Comparison of various *hp***–AMR strategies**

- Comparison of *different hp strategies* for choosing between h and p refinement (2D case)
- AMR cells selection criterion $E^{FV}(\kappa) > \alpha$, a same spatial mesh for all groups, with





▶ Main criterion for h— or p—refinement: pre-asymptotic/asymptotic p convergence regime

Cea Energy group dependent *h***-AMR**

- ▶ h—AMR on the two extreme cases: one single mesh or G = 33 different meshes
- ▶ *E^{FV}* and *E^R* compared for "driving" the adaptation process
- ▶ both ε_{l^2} and $|k k_h|$ (eigenvalue error) monitored



h-refinement for p = 1 driven by either E^{R} or E^{FV}

- w.r.t. ε_{l^2} : E^R and E^{FV} gives similar results for 1 mesh ; clear difference with G meshes: E^R insufficient; additional dof reduction by a factor of 2 to 3 with E^{FV}
- w.r.t. $|k k_h|$: "counter-performance" with *G* meshes, consistent with results reported in [Goffin et al., 2013] where it is attributed to the interpolation error associated with the fission source \rightarrow what about a k-oriented AMR?

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Summary and perspectives

a "classical" tool in reactor physics to *decompose the variations of a quantity of interest* (e.g. the reactivity $\rho = 1 - \frac{1}{k}$) w.r.t. the *local variations of the parameters* associated with the core configuration (nuclear data, material spatial distribution)

a "classical" tool in reactor physics to *decompose the variations of a quantity of interest* (e.g. the reactivity $\rho = 1 - \frac{1}{k}$) w.r.t. the *local variations of the parameters* associated with the core configuration (nuclear data, material spatial distribution)

"Standard" perturbation formula: ρ variation from configuration *i* to configuration *p* In semi-discrete form

$$\Delta \rho_{\Sigma} = -\frac{\left\langle \underline{\phi}_{i}^{\star}, \left(\Delta \underline{\underline{H}} - \Delta \underline{\underline{\varsigma}} - \frac{1}{k_{p}} \Delta \underline{\underline{F}} \right) \underline{\phi}_{p} \right\rangle_{\mathcal{D}^{G \times N}}}{\left\langle \underline{\underline{F}}_{i}^{\star} \underline{\phi}_{i}^{\star}, \underline{\phi}_{p} \right\rangle_{\mathcal{D}^{G \times N}}}$$

$$- \left\langle \underline{\phi}, \underline{\psi} \right\rangle_{\mathcal{D}^{G \times N}} = \sum_{g=1}^{G} \sum_{n=1}^{N} w_n \left\langle \phi_n^g, \psi_n^g \right\rangle_{\mathcal{D}}$$

- ϕ_i^{\star} is the adjoint flux in configuration *i* and, in particular $\Delta \underline{\underline{H}} = \text{diag} \left[\Delta \overline{\Sigma}_t^g(\vec{r}) \right]_{(g,n)}$

 \rightarrow valid only if same discretization for both $\underline{\phi}_i^{\star}$ and $\underline{\phi}_p$ *i.e.* upwind DG: $\underline{\phi}_i, \underline{\phi}_p \in (V_h^{\mathbf{p}})^{G \times N}$

a "classical" tool in reactor physics to *decompose the variations of a quantity of interest* (e.g. the reactivity $\rho = 1 - \frac{1}{k}$) w.r.t. the *local variations of the parameters* associated with the core configuration (nuclear data, material spatial distribution)

- "Standard" perturbation formula: ρ variation from configuration i to configuration p
- ► In the DG framework, this formula extended as $\Delta \rho^{hh'} = \Delta \rho_{\Sigma}^{hh'} + \Delta \rho_{\mathcal{M}}^{hh'}$ [Le Tellier et al., 2011]
- an extra term $\Delta \rho_{\mathcal{M}}^{hh'}$ when $\underline{\phi}_i \in (V_h^{\mathbf{p}})^{G \times N}$ and $\underline{\phi}_p \in (V_{h'}^{\mathbf{p}'})^{G \times N}$
- in particular, if $V_h^{\mathbf{p}}$ is a refinement of $V_{h'}^{\mathbf{p}'}$, it can be written as:

$$\Delta \rho^{hh'} = -\frac{\left\langle \pi_{h'} \underline{\phi}_{i,h}^{\star}, \underline{\phi}_{\rho,h'} \right\rangle_{\mathcal{B}_{h'-}^{G\times N}} - \left\langle \underline{\phi}_{i,h}^{\star}, \pi_{h} \underline{\phi}_{\rho,h'} \right\rangle_{\mathcal{B}_{h-}^{G\times N}}}{\left\langle \underline{F}_{i,h}^{\star} \underline{\phi}_{i,h}^{\star}, \underline{\phi}_{\rho,h'} \right\rangle_{\mathcal{D}^{G\times N}}}$$

- π_h (resp. $\pi_{h'}$), the L^2 -projector on $V_h^{\mathbf{p}}$ (resp. $V_{h'}^{\mathbf{p}'}$),
- $\vec{\nabla}_{hh'}$, the broken gradient operator on the union mesh between \mathcal{M}_h and $\mathcal{M}_{h'}$,

$$\left\langle \underline{\varphi}_{h}, \underline{\phi}_{h} \right\rangle_{\mathcal{B}_{h-}^{G \times N}} = \sum_{g=1}^{G} \sum_{n=1}^{N} w_{n} \sum_{\kappa \in \mathcal{M}_{h}} \left\langle \varphi_{h,n}^{g}, \left[\!\left[\varphi_{h,n}^{g} \right]\!\right] \right\rangle_{\partial \kappa_{-}}$$

a "classical" tool in reactor physics to *decompose the variations of a quantity of interest* (e.g. the reactivity $\rho = 1 - \frac{1}{k}$) w.r.t. the *local variations of the parameters* associated with the core configuration (nuclear data, material spatial distribution)

- **Standard** *perturbation formula*: *ρ variation* from configuration *i* to configuration *p*
- ► In the DG framework, this formula extended as $\Delta \rho^{hh'} = \Delta \rho_{\Sigma}^{hh'} + \Delta \rho_{\mathcal{M}}^{hh'}$ [Le Tellier et al., 2011]
- a priori, this extended formula can be practically useful in two different ways...

Cea AMR and Perturbation theory

► Evaluating the reactivity effect associated with a modification of the "physical" parameters : Improve the AMR performance when evaluating a "physical" reactivity change



Scalar fluxes - configuration "rod in"

for AMR to be fully interesting when evaluating a reactivity worth, $\Delta \rho_{\Sigma}^{hh'}$ to be used instead of $\Delta \rho^{hh'}$



Error on the rod reactivity "worth" - h-refinement

- "direct-driven" (DD) : AMR for direct problem and meshes imposed for adjoint problem
- "adjoint-driven" (AD) : AMR for adjoint problem and meshes imposed for adjoint problem
- "configuration-dependent" (CD) : independent AMR for direct and adjoint problems

AMR and Perturbation theory

Evaluating the change in reactivity due to a mesh refinement: owards a "ρ-oriented" mesh adaptation?

- "two-mesh" error estimators: E^{2M} (flux difference) and E_{ρ}^{2M} ($\Delta \rho^{hh'}$ decomposition over the mesh)
- h-refinement on the ZONA2B benchmark (2D case) with different estimators



No significant gain on ρ convergence when using a ρ error estimator vs. a flux error estimator
 Consistent with the results reported in [Owens et al., 2017] where the more standard "Dual
 Weighted Residual" approach (firstly used in neutronics in [Lathouwers, 2011]) is used

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Cea Summary and perspectives

Summary

- "Sodium Fast Reactors" core physics, ASTRID industrial project
- ▶ Investigation of hp—*AMR* for reducing the burden of solving the neutron transport (Multigroup, S_N , DG upwing scheme)
- Two different error estimators/indicators under very different regularity hypotheses
- ▶ Importance of the *pre-asymptotic/asymptotic p−convergence regime* on dofs reduction
- Connecting the classical "perturbation theory" in reactor core physics with AMR

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And beyond

- ► AMR with DG upwind on *polygonal meshes* (using "non polynomial" element bases → D. Labeurthre ongoing Ph.D. thesis with A. Calloo)
- Performance optimization:
 - Acceleration of these nested iterative loops by a simplified operator (e.g. diffusion) based preconditioning (so-called "Diffusion Synthetic acceleration")
 - Nested iterative loops for solving the source-flux dependency → where to put the AMR loop?
- Energy-space coupling:
 - "Adaptive" condensed energy mesh for group-wise spatial mesh adaptation
 - Spatial domain decomposition with subdomain-dependent energy meshes

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Thank you for your attention

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