Facets Applied Mathematics Group Meetings: Focus on core transport and coupling

Ammar H. Hakim

Facets Winter Meeting, Feb 24th 2011

Agenda is to collaborate effectively with AM/CS folks

We usually meet every Thursday at noon Mountain time.

- Main participants: Lois, Sean, Mike, Brendan, Tom E, Scott Kruger, Srinath, Johan, Alex Pletzer and Ammar.
- We have a mailing list (`facets-am@ice.txcorp.com`) which anyone can join.
- We have a repo (`https://ice.txcorp.com/svnrepos/collabs/facetscollab2011/facets-am`) with slides and notes.
- Aim is to familiarize AM/CS folks with basic equations we wish to solve, develop model problems and, in turn, learn about solvers and coupling strategies.
- Focus on the last several months was on (a) developing an improved core solver, (b) exploring coupling schemes.

One of the more useful and productive meetings.

Agenda is to collaborate effectively with AM/CS folks

We usually meet every Thursday at noon Mountain time.

- Main participants: Lois, Sean, Mike, Brendan, Tom E, Scott Kruger, Srinath, Johan, Alex Pletzer and Ammar.
- We have a mailing list (`facets-am@ice.txcorp.com`) which anyone can join.
- We have a repo (`https://ice.txcorp.com/svnrepos/collabs/facetscollab2011/facets-am`) with slides and notes.
- Aim is to familiarize AM/CS folks with basic equations we wish to solve, develop model problems and, in turn, learn about solvers and coupling strategies.
- Focus on the last several months was on (a) developing an improved core solver, (b) exploring coupling schemes.

One of the more useful and productive meetings.

Agenda is to collaborate effectively with AM/CS folks

We usually meet every Thursday at noon Mountain time.

- Main participants: Lois, Sean, Mike, Brendan, Tom E, Scott Kruger, Srinath, Johan, Alex Pletzer and Ammar.
- We have a mailing list (`facets-am@ice.txcorp.com`) which anyone can join.
- We have a repo (`https://ice.txcorp.com/svnrepos/collabs/facetscollab2011/facets-am`) with slides and notes.
- Aim is to familiarize AM/CS folks with basic equations we wish to solve, develop model problems and, in turn, learn about solvers and coupling strategies.
- Focus on the last several months was on (a) developing an improved core solver, (b) exploring coupling schemes.

One of the more useful and productive meetings.

We have discussed various topics with impact on code in FACETS

- Kruger. Core equations including momentum transport and dynamic equilibrium
- Ammar. Tutorial on how to write FACETS input files
- Ammar. Tutorial on how to create a new FACETS updater to implement an algorithm
- Brendan. Exploring various explicit/implicit coupling schemes for model problems. Done in Matlab, now moving to FACETS
- Pletzer. Errors due to sudden grid resolution changes across core-edge interface
- Mike. Use of PetSc Time-Stepper (TS) layer to write solvers and coupling schemes
- Ammar. Overview of improved core solver input files

Several AM/CS talks and discussions are planned for this meeting: reflects important tasks for FACETS to complete this year

- Tom Epperly on load balancing algorithm using mixed integer linear programming techniques (now in FACETS!).
- Johan and Ammar on an improved core solver design, including dynamic equilibrium, momentum equation and embedded turbulence.
- Brendan on his research on coupling schemes.
- Scott Kruger on getting dynamic equilibrium into FACETS.

Future AM/CS topics: equilibrium formulation, edge equations and edge turbulence transport coupling problems.

Several AM/CS talks and discussions are planned for this meeting: reflects important tasks for FACETS to complete this year

- Tom Epperly on load balancing algorithm using mixed integer linear programming techniques (now in FACETS!).
- Johan and Ammar on an improved core solver design, including dynamic equilibrium, momentum equation and embedded turbulence.
- Brendan on his research on coupling schemes.
- Scott Kruger on getting dynamic equilibrium into FACETS.

Future AM/CS topics: equilibrium formulation, edge equations and edge turbulence transport coupling problems.

We are interested in solving transport equations either stand-alone or coupled to each other

Consider the one-dimensional system of m balance laws

$$\frac{\partial \mathbf{Q}}{\partial t} + \frac{\partial \mathbf{F}}{\partial x} = \mathbf{S}$$

Here $0 < x < x_e$, $\mathbf{Q}(x,t) \in \mathbb{R}^m$, $\mathbf{F}(\mathbf{Q}, \partial\mathbf{Q}/\partial x)$ is the flux $\mathbf{S}(\mathbf{Q}, x, t)$ are source terms.

- Boundary conditions $\mathbf{F} = 0$ at $x = 0$ and either $\mathbf{Q}$ or $\mathbf{F}$ is specified at $x = x_e$.

Details on core discretization in my core solver talk.

We are interested in solving transport equations either stand-alone or coupled to each other

Consider the one-dimensional system of m balance laws

$$\frac{\partial \mathbf{Q}}{\partial t} + \frac{\partial \mathbf{F}}{\partial x} = \mathbf{S}$$

Here $0 < x < x_e$, $\mathbf{Q}(x,t) \in \mathbb{R}^m$, $\mathbf{F}(\mathbf{Q}, \partial \mathbf{Q}/\partial x)$ is the flux $\mathbf{S}(\mathbf{Q}, x, t)$ are source terms.

- Boundary conditions $\mathbf{F} = 0$ at $x = 0$ and either $\mathbf{Q}$ or $\mathbf{F}$ is specified at $x = x_e$.

Details on core discretization in my core solver talk.

We are interested in solving transport equations either stand-alone or coupled to each other

Consider the one-dimensional system of m balance laws

$$\frac{\partial \mathbf{Q}}{\partial t} + \frac{\partial \mathbf{F}}{\partial x} = \mathbf{S}$$

Here $0 < x < x_e$, $\mathbf{Q}(x,t) \in \mathbb{R}^m$, $\mathbf{F}(\mathbf{Q}, \partial \mathbf{Q}/\partial x)$ is the flux $\mathbf{S}(\mathbf{Q}, x, t)$ are source terms.

- Boundary conditions $\mathbf{F} = 0$ at $x = 0$ and either $\mathbf{Q}$ or $\mathbf{F}$ is specified at $x = x_e$.

Details on core discretization in my core solver talk.

We studied coupling algorithms

Imagine solving the transport equation separately on $x < x_c$ and $x > x_c$, where $0 < x_c < x_e$ is a coupling point. We must enforce continuity of values and fluxes

Lemma

Let $0 < x_c < x_e$. Then $\mathbf{Q}(x,t)$ is a solution to the transport equation in $[0, x_e]$ if it is a smooth solution in $x < x_c$ and $x > x_c$ and satisfies the conditions

$$\mathbf{Q}_- = \mathbf{Q}_+$$
$$\mathbf{F}_- = \mathbf{F}_+$$

where $\mathbf{Q}_\pm \equiv \lim_{\epsilon \to 0} \mathbf{Q}(x_c \pm \epsilon, t)$ and $\mathbf{F}_\pm \equiv \mathbf{F}(\mathbf{Q}_\pm, \partial \mathbf{Q}_\pm / \partial x)$.

We studied coupling algorithms

Imagine solving the transport equation separately on $x < x_c$ and $x > x_c$, where $0 < x_c < x_e$ is a coupling point. We must enforce continuity of values and fluxes

Lemma

Let $0 < x_c < x_e$. Then $\mathbf{Q}(x,t)$ is a solution to the transport equation in $[0, x_e]$ if it is a smooth solution in $x < x_c$ and $x > x_c$ and satisfies the conditions

$$\mathbf{Q}_- = \mathbf{Q}_+$$
$$\mathbf{F}_- = \mathbf{F}_+$$

where $\mathbf{Q}_\pm \equiv \lim_{\epsilon \to 0} \mathbf{Q}(x_c \pm \epsilon, t)$ and $\mathbf{F}_\pm \equiv \mathbf{F}(\mathbf{Q}_\pm, \partial \mathbf{Q}_\pm / \partial x)$.

Coupling problem can be stated and solved in multiple ways

Implicit coupling is needed

Transport/free-boundary equilibrium coupling needs to be implicit for stability. Core/edge coupling needs to be implicit for efficiency. What about edge/wall? Core/source?

Different coupling algorithms require different amounts of *intrusive* access to the sub-problem solvers ("components").

- Expose the complete residual of each sub-problem. Requires most intrusive access.
- Treat each sub-problem as a "black box". Requires least intrusive access.
- Some combination of the above two.

Does a particular choice affect *convergence and accuracy* of coupled system?

Coupling problem can be stated and solved in multiple ways

Implicit coupling is needed

Transport/free-boundary equilibrium coupling needs to be implicit for stability. Core/edge coupling needs to be implicit for efficiency. What about edge/wall? Core/source?

Different coupling algorithms require different amounts of *intrusive* access to the sub-problem solvers ("components").

- Expose the complete residual of each sub-problem. Requires most intrusive access.
- Treat each sub-problem as a "black box". Requires least intrusive access.
- Some combination of the above two.

Does a particular choice affect *convergence and accuracy* of coupled system?

Coupling problem can be stated and solved in multiple ways

Implicit coupling is needed

Transport/free-boundary equilibrium coupling needs to be implicit for stability. Core/edge coupling needs to be implicit for efficiency. What about edge/wall? Core/source?

Different coupling algorithms require different amounts of *intrusive* access to the sub-problem solvers ("components").

- Expose the complete residual of each sub-problem. Requires most intrusive access.
- Treat each sub-problem as a "black box". Requires least intrusive access.
- Some combination of the above two.

Does a particular choice affect *convergence and accuracy* of coupled system?

Coupling problem can be stated and solved in multiple ways

Implicit coupling is needed

Transport/free-boundary equilibrium coupling needs to be implicit for stability. Core/edge coupling needs to be implicit for efficiency. What about edge/wall? Core/source?

Different coupling algorithms require different amounts of *intrusive* access to the sub-problem solvers ("components").

- Expose the complete residual of each sub-problem. Requires most intrusive access.
- Treat each sub-problem as a "black box". Requires least intrusive access.
- Some combination of the above two.

Does a particular choice affect *convergence and accuracy* of coupled system?

Coupling problem can be stated and solved in multiple ways

Implicit coupling is needed

Transport/free-boundary equilibrium coupling needs to be implicit for stability. Core/edge coupling needs to be implicit for efficiency. What about edge/wall? Core/source?

Different coupling algorithms require different amounts of *intrusive* access to the sub-problem solvers ("components").

- Expose the complete residual of each sub-problem. Requires most intrusive access.
- Treat each sub-problem as a "black box". Requires least intrusive access.
- Some combination of the above two.

Does a particular choice affect *convergence and accuracy* of coupled system?

Intrusive implicit coupling requires full access to sub-problem residuals

We can schematically write the sub-problems as

$$\mathbf{U} = \mathcal{U}(\mathbf{U}, \mathbf{v})$$
$$\mathbf{V} = \mathcal{V}(\mathbf{V}, \mathbf{u})$$

where $\mathbf{U}$ is vector of unknowns for first sub-problem and $\mathbf{V}$ is the vector of unknowns for second sub-problem. The variables $\mathbf{u}$ and $\mathbf{u}$ represent coupling variables.

$$\mathbf{u} = \overline{\mathcal{U}}(\mathbf{U})$$
$$\mathbf{v} = \overline{\mathcal{V}}(\mathbf{V})$$

In words: the coupling variables $\mathbf{u}$ are some function of internal variables $\mathbf{U}$ of first sub-problem. Ditto for $\mathbf{v}$.

Intrusive implicit coupling requires full access to sub-problem residuals

We can schematically write the sub-problems as

$$\mathbf{U} = \mathcal{U}(\mathbf{U}, \mathbf{v})$$
$$\mathbf{V} = \mathcal{V}(\mathbf{V}, \mathbf{u})$$

where **U** is vector of unknowns for first sub-problem and **V** is the vector of unknowns for second sub-problem. The variables **u** and **u** represent coupling variables.

$$\mathbf{u} = \overline{\mathcal{U}}(\mathbf{U})$$
$$\mathbf{v} = \overline{\mathcal{V}}(\mathbf{V})$$

In words: the coupling variables **u** are some function of internal variables **U** of first sub-problem. Ditto for **v**.

Intrusive implicit coupling requires full access to sub-problem residuals II

For *explicit* coupling we have iterative scheme

$$\mathbf{U}^{k+1} = \mathcal{U}(\mathbf{U}^{k+1}, \mathbf{v}^k)$$
$$\mathbf{V}^{k+1} = \mathcal{V}(\mathbf{V}^{k+1}, \mathbf{u}^k)$$

i.e. coupling variables are computed for *previous* iterate. For *implicit* coupling we need to approximate the Jacobian

$$\mathbf{J} = \begin{bmatrix} \mathbf{I} - \partial\mathcal{U}/\partial\mathbf{U} & 0 & 0 & -\partial\mathcal{U}/\partial\mathbf{v} \\ 0 & \mathbf{I} - \partial\mathcal{V}/\partial\mathbf{V} & -\partial\mathcal{V}/\partial\mathbf{u} & 0 \\ -\partial\overline{\mathcal{U}}/\partial\mathbf{U} & 0 & \mathbf{I} & 0 \\ 0 & -\partial\overline{\mathcal{V}}/\partial\mathbf{V} & 0 & \mathbf{I} \end{bmatrix}$$

Intrusive implicit coupling requires full access to sub-problem residuals II

For *explicit* coupling we have iterative scheme

$$\mathbf{U}^{k+1} = \mathcal{U}(\mathbf{U}^{k+1}, \mathbf{v}^k)$$
$$\mathbf{V}^{k+1} = \mathcal{V}(\mathbf{V}^{k+1}, \mathbf{u}^k)$$

i.e. coupling variables are computed for *previous* iterate. For *implicit* coupling we need to approximate the Jacobian

$$\mathbf{J} = \begin{bmatrix} \mathbf{I} - \partial\mathcal{U}/\partial\mathbf{U} & 0 & 0 & -\partial\mathcal{U}/\partial\mathbf{v} \\ 0 & \mathbf{I} - \partial\mathcal{V}/\partial\mathbf{V} & -\partial\mathcal{V}/\partial\mathbf{u} & 0 \\ -\partial\overline{\mathcal{U}}/\partial\mathbf{U} & 0 & \mathbf{I} & 0 \\ 0 & -\partial\overline{\mathcal{V}}/\partial\mathbf{V} & 0 & \mathbf{I} \end{bmatrix}$$

Black-box implicit coupling does not require any knowledge of sub-problem internals

We can schematically write the coupling problem as

$$\mathbf{u} = \overline{\mathcal{U}}(\mathbf{v})$$
$$\mathbf{v} = \overline{\mathcal{V}}(\mathbf{u})$$

In words: consider the *first* sub-problem as a "black" box that takes in coupling variables computed in the *second* sub-problem. Now we need to approximate the *smaller* Jacobian

$$\mathbf{J} = \begin{bmatrix} \mathbf{I} & -\partial\overline{\mathcal{U}}/\partial\mathbf{v} \\ -\partial\overline{\mathcal{V}}/\partial\mathbf{u} & \mathbf{I} \end{bmatrix}$$

Can PetSc TS objects be used for such coupling schemes? (See Mike's Facets-AM talk in repo)

Black-box implicit coupling does not require any knowledge of sub-problem internals

We can schematically write the coupling problem as

$$\mathbf{u} = \overline{\mathcal{U}}(\mathbf{v})$$
$$\mathbf{v} = \overline{\mathcal{V}}(\mathbf{u})$$

In words: consider the *first* sub-problem as a “black” box that takes in coupling variables computed in the *second* sub-problem. Now we need to approximate the *smaller* Jacobian

$$\mathbf{J} = \begin{bmatrix} \mathbf{I} & -\partial\overline{\mathcal{U}}/\partial\mathbf{v} \\ -\partial\overline{\mathcal{V}}/\partial\mathbf{u} & \mathbf{I} \end{bmatrix}$$

Can PetSc TS objects be used for such coupling schemes? (See Mike's Facets-AM talk in repo)

Black-box implicit coupling does not require any knowledge of sub-problem internals

We can schematically write the coupling problem as

$$\mathbf{u} = \overline{\mathcal{U}}(\mathbf{v})$$
$$\mathbf{v} = \overline{\mathcal{V}}(\mathbf{u})$$

In words: consider the *first* sub-problem as a "black" box that takes in coupling variables computed in the *second* sub-problem. Now we need to approximate the *smaller* Jacobian

$$\mathbf{J} = \begin{bmatrix} \mathbf{I} & -\partial\overline{\mathcal{U}}/\partial\mathbf{v} \\ -\partial\overline{\mathcal{V}}/\partial\mathbf{u} & \mathbf{I} \end{bmatrix}$$

Can PetSc TS objects be used for such coupling schemes? (See Mike's Facets-AM talk in repo)

Outstanding issues and current work

- What is the effect of grid mis-match and sudden resolution changes on surfacial coupling schemes? Alex has done some initial work in 1D for a test problem, need to build upon.
- What is the "correct" formulation of interface updates to ensure we are solving the *same* problem when we do coupling versus doing the whole problem in a single domain? (Brendan's talk today).
- What happens for volumetric coupling when the grids do not overlap?
- What is the efficiency and accuracy of coupled explicit/implicit solvers when the models do not exactly match up?
- What is the effect of initialization errors on early time behaviour of the coupled system evolution?
- What is the general software infrastructure to have reusable suite of coupling schemes?

Outstanding issues and current work

- What is the effect of grid mis-match and sudden resolution changes on surfacial coupling schemes? Alex has done some initial work in 1D for a test problem, need to build upon.
- What is the "correct" formulation of interface updates to ensure we are solving the *same* problem when we do coupling versus doing the whole problem in a single domain? (Brendan's talk today).
- What happens for volumetric coupling when the grids do not overlap?
- What is the efficiency and accuracy of coupled explicit/implicit solvers when the models do not exactly match up?
- What is the effect of initialization errors on early time behaviour of the coupled system evolution?
- What is the general software infrastructure to have reusable suite of coupling schemes?

Outstanding issues and current work

- What is the effect of grid mis-match and sudden resolution changes on surfacial coupling schemes? Alex has done some initial work in 1D for a test problem, need to build upon.
- What is the "correct" formulation of interface updates to ensure we are solving the *same* problem when we do coupling versus doing the whole problem in a single domain? (Brendan's talk today).
- What happens for volumetric coupling when the grids do not overlap?
- What is the efficiency and accuracy of coupled explicit/implicit solvers when the models do not exactly match up?
- What is the effect of initialization errors on early time behaviour of the coupled system evolution?
- What is the general software infrastructure to have reusable suite of coupling schemes?

Outstanding issues and current work

- What is the effect of grid mis-match and sudden resolution changes on surfacial coupling schemes? Alex has done some initial work in 1D for a test problem, need to build upon.
- What is the "correct" formulation of interface updates to ensure we are solving the *same* problem when we do coupling versus doing the whole problem in a single domain? (Brendan's talk today).
- What happens for volumetric coupling when the grids do not overlap?
- What is the efficiency and accuracy of coupled explicit/implicit solvers when the models do not exactly match up?
- What is the effect of initialization errors on early time behaviour of the coupled system evolution?
- What is the general software infrastructure to have reusable suite of coupling schemes?

Outstanding issues and current work

- What is the effect of grid mis-match and sudden resolution changes on surfacial coupling schemes? Alex has done some initial work in 1D for a test problem, need to build upon.
- What is the "correct" formulation of interface updates to ensure we are solving the *same* problem when we do coupling versus doing the whole problem in a single domain? (Brendan's talk today).
- What happens for volumetric coupling when the grids do not overlap?
- What is the efficiency and accuracy of coupled explicit/implicit solvers when the models do not exactly match up?
- What is the effect of initialization errors on early time behaviour of the coupled system evolution?
- What is the general software infrastructure to have reusable suite of coupling schemes?

Outstanding issues and current work

- What is the effect of grid mis-match and sudden resolution changes on surfacial coupling schemes? Alex has done some initial work in 1D for a test problem, need to build upon.
- What is the "correct" formulation of interface updates to ensure we are solving the *same* problem when we do coupling versus doing the whole problem in a single domain? (Brendan's talk today).
- What happens for volumetric coupling when the grids do not overlap?
- What is the efficiency and accuracy of coupled explicit/implicit solvers when the models do not exactly match up?
- What is the effect of initialization errors on early time behaviour of the coupled system evolution?
- What is the general software infrastructure to have reusable suite of coupling schemes?