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First Steps Toward a Multiphysics Exemplars and Benchmarks Suite

Mathematics and Computer Science Division

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Preliminary Ideas from the 2011 ICiS Workshop on *Multiphysics Simulations: Challenges and Opportunities*

A workshop report (**Keyes et al., 2012**) summarizes challenges and opporunities in multiphysics simulations from algorithmic and architectural perspectives, where "algorithmic" includes both mathematical analysis and computational complexity and "architectural" includes both software and hardware environments. The report discusses the significant and still remaining key needs for conducting the mathematical analysis and developing the corresponding flexible software necessary to ensure that coupling schemes are accurate, stable, robust, consistent, and are implemented correctly, as prerequisites for developing predictive multiphysics simulations. Such work is essential for exploiting emerging extreme-scale computing resources for scientific discovery.

A collection of multiphysics exemplars and benchmarks that encompass features present in many applications would provide a resource for motivating and validating new research on multiphysics algorithms and software. Goals of an overall collection include diversity of mathematical formulation (e.g., fields and particles), simplicity of code size to describe, range of scale and parametric challenge, and range of applicability to different user communities. Initial pointers to multiphysics test problems collected during the 2011 ICiS Multiphysics Workshop are available via the workshop website (**Keyes et al., 2011**).

This document takes a first step at presenting a few multiphysics exemplars in a unified format, based on that used by **Kamm et al. (2008)**, though with a few modifications to convey additional information that we consider relevant in multiphysics contexts. A longer-term goal is to engage the community to contribute a broader range of representative multiphysics test cases and codes that could be published on a webpage that outlives an archival fixed publication and could be updated from time to time. We initially consider the following examples:

- **Advection-reaction** (1): This example is a prototypical reactive transport problem, and it is a good test for the convergence of IMEX time integration schemes and order reduction phenomena due to stiffness.
- **Heat transfer coupled across an interface** (2): A simple linear heat equation with constant diffusivity is posed on two neighboring, non-overlapping subdomains that meet along an interface.
- **Conjugate heat transfer** (3): This example illustrates the flow of a fluid around a cylinder of a different temperature, where the regions are coupled through the heat equations by continuity of state and normal flux. The flow of the fluid guarantees that the effects of error are felt downstream from the object. Coupling can be handled in various ways. Note that in general there will be different methods for the fluid equations and the heat equations, providing another difficulty.

1 Advection-reaction

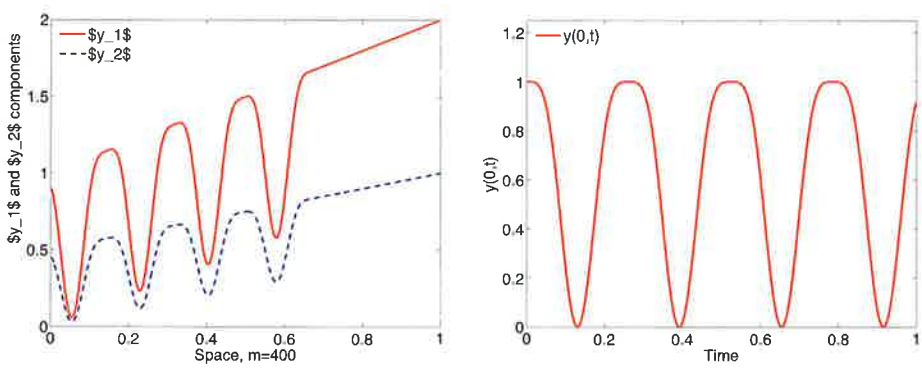
- **Contributor:** Emil Constantinescu, Argonne National Laboratory
- **Conceptual Description**
  - **General:** This is a typical reactive-transport problem exposing two physical processes that share the same spatial domain: advection and a linear kinetic process. The two processes have different temporal scales—the advection process is relatively slow, whereas the kinetic term is numerically stiff. Therefore, this problem is suitable for partitioned time integration methods and, in particular, IMEX schemes as discussed in Section 3.2.2 of (Keyes et al., 2012). This problem can be made very stiff, in which case the order reduction phenomenon and stiffness leakage can be analyzed. The governing equations model the dynamics of two chemical species by

$$\begin{aligned} \frac{\partial y_1}{\partial t} + \alpha_1 \frac{\partial y_1}{\partial x} &= -k_1 y_1 + k_2 y_2 + s_1 \\ \frac{\partial y_2}{\partial t} + \alpha_2 \frac{\partial y_2}{\partial x} &= k_1 y_1 - k_2 y_2 + s_2 \,. \end{aligned}$$

  - **Processes modeled:** advective transport and chemical kinetics on the same spatial domain. We can write the problem as $y' = f(y) + g(y)$, where f represents advection and g (possibly stiff) reaction. The solution at $t = 1$ is illustrated in Figure 1.a.
  - **Specification of initial conditions:**

$$y_1(x,0) = 1 + s_2 x\,,\; y_2(x,0) = \frac{k_1}{k_2} y_1(x,0) + \frac{1}{k_2} s_2$$

  - **Specification of boundary conditions:** $y_1(0,t) = 1 - \sin(12t)^4$ (see Fig. 1.b). The right boundary condition is an outflow boundary. If $\alpha_2 = 0$, then there is no need to specify boundary conditions for the second component.
  - **Benchmark type:** convergence of time integration strategies and order reduction.
  - **Description of quantities in which accuracy is important:** For convergence analysis, all quantities are important in this problem. However, one may consider different quantities of interest, such as the total mass of one of the species.



(a) Solution at $t = 1$ (b) Inflow function

Figure 1: Illustration of (a) the advection-reaction solution and (b) the boundary inflow term ($y_1(0,t)$).

- **Principal Features Tested**
  - **Discretization:** This test is aimed at temporal discretization, Thus, we provide a simple, high-order (order 4) spatial discretization that can be used with this example. The spatial grid is defined as $x_i = i\Delta x$, $i = 1 \ldots m$, $\Delta x = 1/m$; and the advective term can be discretized as

$$
\begin{aligned}
f(x_1) &= \alpha\frac{1}{\Delta x}\left(\frac{1}{3}y(0,t) + \frac{1}{2}y(x_1) - y(x_2) + \frac{1}{6}y(x_3)\right)\\
f(x_2) &= \alpha\frac{1}{\Delta x}\left(-\frac{1}{12}y(0,t) + \frac{2}{3}y(x_1) - \frac{2}{3}y(x_3) + \frac{1}{12}y(x_4)\right)\\
f(x_j) &= \alpha\frac{1}{\Delta x}\left(-\frac{1}{12}y(x_{j-2}) + \frac{2}{3}y(x_{j-1}) - \frac{2}{3}y(x_{j+1}) + \frac{1}{12}y(x_{j+2})\right)\ ,\ j = 3\ldots m-2\\
f(x_{m-1}) &= \alpha\frac{1}{\Delta x}\left(-\frac{1}{6}y(x_{m-3}) + y(x_{m-2}) - \frac{1}{2}y(x_{m-1}) - \frac{1}{3}y(x_m)\right)\\
f(x_m) &= \alpha\frac{1}{\Delta x}\left(-y(x_m) + y(x_{m-1})\right).
\end{aligned}
$$

  - **Algorithms:** This problem can be integrated in time with a fully implicit method as well as a partitioned method in which f is integrated with an explicit integrator and g with an implicit one.
  - **Solver:** Multiple solvers can be used to test different aspects related to algorithmic efficiency and effectiveness. However, because this problem is a small-scale experiment, convergence and relative implementation and computational cost between fully implicit and IMEX methods can be explored.
  - **Code:** The code can be easily implemented in Matlab. It is implemented in PETSc (which allows a simple switch between fully implicit and IMEX using additive Runge-Kutta schemes).
- **Mathematical Description**
  - **Problem domain:** This is a one-dimensional experiment with $m = 400$ grid points for each component. The problem domain is delimited by

$$0 < x < 1\,, \qquad 0 < t \leqslant t_{\max}\,.$$

  - **Ranges of data and parameters:** Typical ranges for the parameters that yield a stiff problem are

$$
\begin{aligned}
\alpha_1 &= 1,\ k_1 = 10^6,\ s_1 = 0,\\
\alpha_2 &= 0,\ k_2 = 2k_1,\ s_2 = 1\,.
\end{aligned}
$$

- **Accuracy Assessment:** A reference solution can be computed by using a small timestep with classical stiff integrators.
- **Testing Procedures:** The stability and accuracy testing procedure (i.e., the convergence and its rate) can be achieved by measuring the error when using different time steps. For multistage methods (Runge-Kutta) the convergence rate beyond a certain error level may drop to the method's stage order—the order reduction phenomenon. Fully implicit methods suffer from the same peril.
- **Additional User Information:** When using nonlinear discretization schemes for f (shock-capturing schemes (e.g., flux-limited WENO), it is convenient to employ an IMEX procedure that does not need a Jacobian approximation of this component. Moreover, by using a splitting strategy one can take advantage of the fact that the stiff (implicitly integrated) component is linear and does not require nonlinear solves.
- **References:** (Hundsdorfer and Ruuth, 2007; Constantinescu and Sandu, 2010); contact Emil Constantinescu (`emconsta@mcs.anl.gov`).

2 Heat transfer coupled across an interface

- **Contributor:** Brendan Sheehan, Colorado State University
- **Conceptual Description**
  - **General:** A simple linear heat equation with constant diffusivity is posed on two neighboring, non-overlapping subdomains that meet along an interface. Equality of state and normal flux are enforced along the interface. The subscripts "c" and "e" stand for core and edge and are used below to differentiate the subdomains.

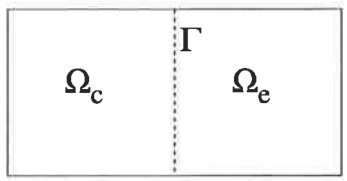


Figure 2: Illustration of neighboring subdomains

$$
\begin{aligned}
\frac{\partial}{\partial t}\mathcal{U}_c - \nabla\cdot(\nabla\mathcal{U}_c) &= \mathcal{S}_c \quad \text{on } \Omega_c \\
\frac{\partial}{\partial t}\mathcal{U}_e - \nabla\cdot(\nabla\mathcal{U}_e) &= \mathcal{S}_e \quad \text{on } \Omega_e \\
\mathcal{U}_c &= \mathcal{U}_e \quad \text{on } \Gamma \\
\hat{n}\cdot\nabla\mathcal{U}_c &= \hat{n}\cdot\nabla\mathcal{U}_e \quad \text{on } \Gamma
\end{aligned}
$$

  - **Processes modeled:** The only physics modeled is heat transfer, but it is the error caused by the exchange of information across the interface that is of interest.
  - **Specification of initial conditions:** Each subdomain requires a standard initial condition $U_0 = U(\vec{x}, t)\,|_{t=0}$.
  - **Specification of boundary conditions:** Each subdomain requires standard Dirichlet or Neumann boundary conditions on $\Omega_c\backslash\Gamma$ and $\Omega_e\backslash\Gamma$, respectively.
  - **Benchmark type:** stability and accuracy of coupling algorithms.
  - **Description of quantities in which accuracy is important:** The quantity of interest is the difference between the computed solution and the implicitly coupled solution (see accuracy assessment below), measured in a suitable norm. Special attention is paid to the error near the interface, where inaccuracies often appear and grow in time. Also, the error at the end time of longer simulations is more likely to reveal any instability. One could consider (a) the temperature at the midpoint of one domain at a specific time T and time averaged from 0 to T, and (b) the average spatial temperature over one domain at a specific time T and time averaged from 0 to T.
- **Principal Features Tested**
  - **Discretization:** The discretization within the subdomains is something standard, like finite volume in space and backward Euler in time. The discretization of the interface conditions (equality of state and normal derivative on the interface) can be varied and tested.
  - **Algorithms:** The solution algorithm is a blockwise iterative procedure at each timestep. The two subdomains swap information and are then solved independently. This procedure can be done once at each timestep or repeatedly at each timestep in hopes of converging to a better solution for that timestep.
  - **Solver:** The solver consists of the most accurate direct solve available, with no concern for computational cost. The accuracy and stability issues introduced by the coupling can then be examined without error from inexact solves in the subdomains entering the picture.

- **Code:** Matlab

- **Mathematical Description**
  - **Problem domain:** In 1D, the domain is $x \in [0, 1]$ with the interface between the subdomains at $x = .5$. In 2D the subdomains are two neighboring squares.
  - **Ranges of data and parameters:** The diffusivity is left at a constant equal to one. The forcing term is set to match the manufactured solution. The size of the grid cells, the size of the timestep, and the number of iterations performed at each timestep are the parameters to be varied.

- **Accuracy Assessment:** The problem is constructed by starting with a known continuous solution and calculating the corresponding source term. Two forms of discrete solution are then produced. One, called the implicitly coupled solution, is computed by directly inverting the coupled discrete system. The second, called the computed solution, is computed by performing the block iteration described above at each timestep. The error between these solutions can then be measured directly.

- **Testing Procedures:** The accuracy and stability of the algorithm for various timesteps and numbers of iterations per timestep are tested by direct measurement of error.

- **Additional User Information:** It is also possible to do multirate examples, where the timestep in one subdomain is an integer multiple of the timestep in the other subdomain.

- **References:** Contact Brendan Sheehan (`brendansheehan6@gmail.com`) .

3 Conjugate heat transfer

- **Contributors:** Don Estep and Brendan Sheehan, Colorado State University
- **Conceptual Description**
  - **General:** This is the flow of a fluid around a cylinder of a different temperature, where the regions are coupled through the heat equations by continuity of state and normal flux. The flow of the fluid guarantees that the effects of error are felt downstream from the object.

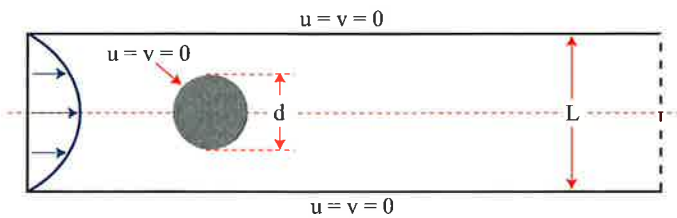


Figure 3: Illustration of conjugate heat transfer problem

$$\begin{cases} -\mu\Delta\mathbf{u} + \rho_0\left(\mathbf{u}\cdot\nabla\right)\mathbf{u} + \nabla p + \rho_0\beta T_F\mathbf{g} = \rho_0\left(1+\beta T_0\right)\mathbf{g}, & x\in\Omega_F, \\ -\nabla\cdot\mathbf{u} = 0, & x\in\Omega_F, \\ -k_F\Delta T_F + \rho_0 c_p(\mathbf{u}\cdot\nabla T_F) = Q_F, & x\in\Omega_F, \\ \begin{cases} T_S = T_F, \\ k_F(\hat{n}\cdot\nabla T_F) = k_S(\hat{n}\cdot\nabla T_S), \end{cases} & x\in\Gamma_I, \\ -k_S\Delta T_S = Q_S, & x\in\Omega_S, \end{cases}$$

The symbols ρ_0 and T_0 are reference values for the density and temperature respectively, μ is the molecular viscosity, β is the coefficient of thermal expansion, c_p is the specific heat, k_F and k_S are the thermal conductivities of the fluid and solid respectively, Q_F and QS are source terms, and $\hat{n}$ is the unit normal vector directed into the fluid.

  - **Processes modeled:** Heat transfer and fluid flow.
  - **Specification of initial conditions:** Not required for steady-state problem; required for time-dependent version.
  - **Specification of boundary conditions:** The fluid subdomain requires a known profile at the inflow boundary and uses a zero velocity condition at the outer walls and at the interface with the solid. The temperature/heat flux boundary conditions must be known on $\partial\Omega_F\backslash\Gamma_I$ and are provided on Γ_I by information exchange between the subdomains. This process starts with the initial conditions in the time-dependent case and requires some initial guess in the steady-state case.
  - **Benchmark type:** Coupling two different PDEs discretized with two different discrete methods, evaluating both stability and accuracy.
  - **Description of quantities in which accuracy is important:** Examples of quantities of interest include the average temperature in the solid, or the temperature at a specific point in the solid, or fluid downstream of the solid. One could consider (a) the temperature at the midpoint of the solid at a specific time T and time averaged from 0 to T, (b) the average spatial temperature over the solid at a specific time T and time averaged from 0 to T, and (c) the temperature in the fluid downstream a small ways from the solid at a specific time T and time averaged from 0 to T.

- **Principal Features Tested**
  - **Discretization:** Different discretizations may be needed for the fluid and solid subdomains, and this is likely to put some stress on the accuracy of the solution.
  - **Algorithm/solver/code:** The subdomains are coupled through an iteration in which temperature and heat flux information is passed from one subdomain to the other. Furthermore, the fluid subdomain has heat transfer coupled to fluid flow. Therefore, either the component solution in the fluid either must come from a solver that can handle this all at once, or an additional iteration between a fluid code and a heat transfer code must take place within the fluid subdomain.
- **Mathematical Description**
  - **Problem domain:** 2D pipe in which the fluid flows.
  - **Ranges of data and parameters:** The material properties of the fluid and solid are the parameters to be varied, including the thermal conductivity of the solid and fluid, and the viscosity of the fluid.
- **Accuracy Assessment/Testing Procedures:** A posteriori error analysis is used to assess the accuracy in a quantity of interest. Alternatively, a reference solution on a very fine grid could be used to assess the accuracy of the solution on a coarse grid.
- **References:** Contact Brendan Sheehan (`brendansheehan6@gmail.com`) .

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