Multi-physics/Multi-Scale Methods I: Methods for Multi-physics Coupled Solvers

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Introduction

My research is primarily concerned with the development of solvers for large-scale multi-physics simulations.

- I focus on implicitly-coupled methods, typically resulting in the solution of large-scale systems of nonlinear equations at each time step.
- Experience in extending legacy codes to include new physics/implicitness.
- Concerned with multi-scale problems in *time*, as opposed to problems with multiple spatial scales [Bangerth, Ghattas, ...].
- Application areas include
  - Fusion: hydrodynamics + electromagnetics
  - Astrophysics: hydrodynamics + radiation transport
  - Cosmology: hydrodynamics + self-gravity + radiation transport + chemical ionization kinetics
  - Materials Science: nonlinear elasticity + thermodynamics

Outline

I. Introduction

II. General Coupling Methods for Multi-physics Solvers
   - Explicit
   - Mixed Explicit & Implicit
   - Implicit

III. Case Studies
   - Magnetic Fusion
   - Cosmic Reionization

Extended Example – Notation

We consider time evolution of a coupled (nonlinear) modeling system,

$$\frac{\partial}{\partial t}U = F(U) + S(U),$$

where U contains the physical variables and F and S represent processes that operate at different speeds, c_{fast} and c_{slow}, respectively, e.g.

- fast chemical reactions coupled with slower global diffusion
- stiff surface gravity waves in climate models
- stiff diffusion processes coupled with non-stiff advection

While many models admit easily-separable components, allowing approximation through a variety of techniques (dropping terms, model reduction, steady-state assumptions), modern science is deriving higher-fidelity models where those simplifications become less clear (nonlinearities, complicated EOS, ...).

Explicitly-Coupled Multi-Physics Methods

Fully explicit, fixed step methods include the forward Euler method:

$$U^{n+1} = U^n + \Delta t \left[F(U^n) + S(U^n) \right].$$

(+) The first approach in many multi-physics codes (simplest).

(+) High order accuracy possible through Runge-Kutta and explicit linear multistep methods.

(−) Δt is limited by the stability of the fastest physical process

$$\Delta t_{CFL} \leq \frac{\Delta x^{\alpha}}{c_{fast}}.$$

(−) Intractable for *stiff* calculations, in which $c_{fast} \gg c_{slow}$ but overall dynamics evolve at c_{slow}.

(−) Cannot scale to very large problems, since $\Delta x \to 0 \;\; \Rightarrow \;\; \Delta t \to 0$.

Multiple Time Step Coupling Methods

Basic multiple time step methods iterate (explicitly) on the fast dynamics. Decomposing $U = (U_f, U_s)$ one may split up the physics to write:

$$U_f{}^{n+(j+1)/k} = U_f{}^{n+j/k} + \Delta t_f \, F\left(U_f{}^{n+j/k}, U_s{}^{n}\right), \quad j = 0, \ldots, k-1$$

$$U_s{}^{n+1} = U_s{}^{n} + \Delta t_s \, S\left(U_f{}^{n+1}, U_s{}^{n}\right).$$

- Typically $\Delta t_s = c\,\Delta t_f$, where c is some positive integer.

(+) Almost as simple as standard explicit methods.

(+) Not all terms need to be evaluated at each step.

(−) Splitting must be determined *a priori*.

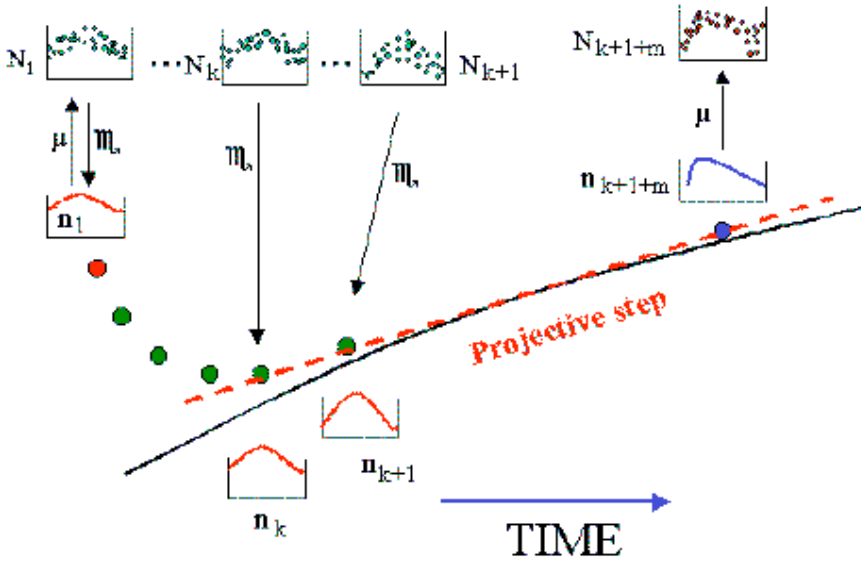
(−) Even if Δt_f and Δt_s adhere to stability restrictions, can result in numerical *resonance instabilities* [Grubmüller 1991; Biesiadecki & Skeel 1993].

Coarse Projective Integration

Developed for problems with unknown microscale→macroscale constitutive laws.

Laws are computed on the fly by integrating the microscale equations directly.

1. *lifting*: create appropriate micro model ICs from macro model.
2. *evolution*: explicitly evolve micro model for some duration.
3. *restriction*: project the detailed solution to macro variables.
4. *projection*: combine multiple micro solutions to take large step.



[Gear et al., *Comp Chem Engrg*, 2002]

May be combined with the *gap-tooth* method for the *patch dynamics* approach.

Advantage lies in applicability to models for which no PDE is (yet) available, e.g. kinetic Monte Carlo and molecular dynamics.

Projective integrators / Gap-Tooth Method: [Gear, Kevrekedis, Theodoropoulos, Lee, Samaey]

Mixed Explicit & Implicit Coupling Methods

Mixed methods treat each component with a different solver, e.g.

$$U^{n+1} = U^n + \Delta t \left[F(U^{n+1}) + S(U^n) \right].$$

- Prototypical "operator splitting", since separated physics enables:
  - leveraging of optimized legacy codes to a common purpose,
  - optimal solvers (e.g. FFT) may be used on individual components,
- F is sometimes split into implicit and explicit parts, typically used so that implicit piece is linear, and remainder is explicit ["linearly-implicit"].
- Requires *a priori* knowledge of easily-separable stiff & nonstiff parts.
- Typically low-order accurate, though higher-order in each component is feasible [*IMEX* methods by Crouzeix 1980; Ascher et al. 1997].
- Often results in numerical instabilities purely due to the splitting that may be difficult to identify/rectify [see talks by John Shadid & Don Estep].

Implicitly-Coupled Methods

Implicitly-coupled approaches treat everything with an implicit method, e.g.

$$U^{n+1} = U^n + \Delta t \left[F(U^{n+1}) + S(U^{n+1}) \right].$$

(−) May result in large-scale nonlinear problems, with possibly undesirable structure (e.g. dense or non-symmetric matrices) $\longrightarrow$ difficult to solve.

(+) May guarantee stability for arbitrary Δt.

(+) Allows high accuracy solutions within *and between* variables.

(+) May be constructed using modern applied math toolkits, e.g. PETSc, SUNDIALS, Trilinos, that

- have come a long way since "Numerical Recipes",
- allow complicated data structures,
- enable specialized solver capabilities and interfaces to some of the most scalable and efficient solver libraries in existence.
- (and they're free)

Implicit Solver Structure

Implicit systems are typically solved using a variant of Newton's method:

- Let $g(U)$ be the vector of all equations to be solved in a time step, e.g.

$$g(U) = U - U^n - \Delta t\,[F(U) + S(U)]\,, \qquad g(U) = 0 \Rightarrow U \approx U(t^{n+1}).$$

- Newton solvers iterate to $\|g(U)\| \leq \varepsilon$ via: set $U_0 \approx U^n$,
  - (i) solve $J(U_k)\delta U_k = -g(U_k)$ where $J(U) = \frac{\partial}{\partial U} g(U)$
  - (ii) update $U_{k+1} = U_k + \lambda_k \delta U_k$ for $0 < \lambda_k \leq 1$
  - $\|\cdot\|$ is a weighted norm, balancing multi-physics components
- Linear solvers for $J\delta U = -g$ are typically iterative:
  - Do not require matrix J, only its *action*, $Jv \approx [g(U + \sigma v) - g(U)]/\sigma$.
  - Amenable to very large scale problems.
  - May be combined with other solvers through *preconditioner/smoother*.

Newton: [Dembo et al. 1982; Kelley 1995; . . .]
Multigrid: [Brandt 1973; *Tuminaro (talk)*; . . .]

Krylov: [Saad & Schultz 1986; Greenbaum 1997; . . .]
Schwarz: [Keyes 1989; Widlund 1989; . . .]

Preconditioning

Preconditioner notes:

- Instead of $J\,\delta U = -g$, you solve $(JP^{-1})(P\delta U) = -g$ or $(P^{-1}J)\,\delta U = -P^{-1}g$.
- Want $P \approx J$ for rapid convergence, but need P^{-1} efficient.
- Inaccuracies in P do not affect the accuracy of the nonlinear solution, only the convergence properties of the linear solver.

Allows domain-specific knowledge back into the solver:

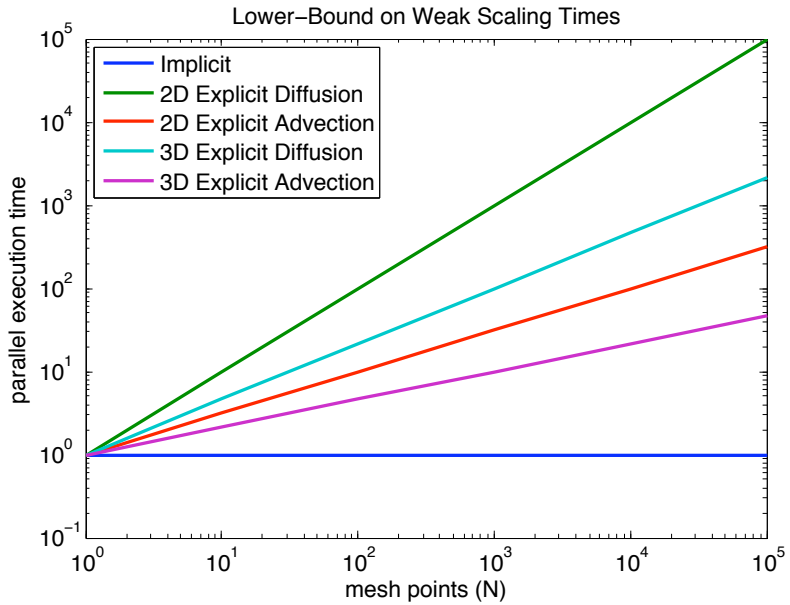
- Any *a priori* knowledge can help $\rightarrow$ may only need to treat stiff parts.
- Operator-split approaches may be used to separately attack different components of $J(U)$, allowing optimal solvers on individual processes.
- Legacy codes can be repurposed as preconditioners.
- Physical approximations (lagging, model reduction, ...) may be incorporated into P, enabling physical intuition while retaining accuracy.

Preconditioning Overview: [Knoll & Keyes 2005]

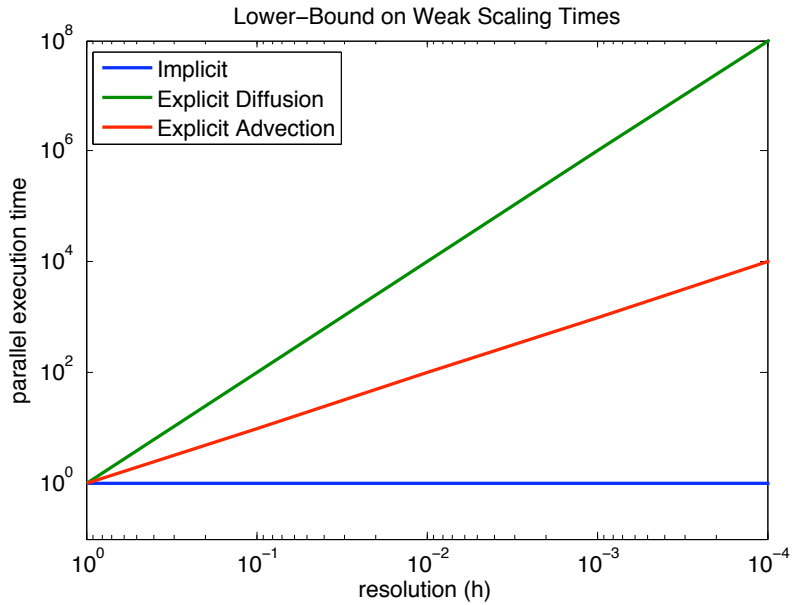
Weak Scaling Limits

Assuming ideal-complexity algorithms ($\mathcal{O}(N)$), quasi-uniform mesh size h, spatial dimension d, and textbook CFL stability criteria, we estimate the *best case* expected time E for weak scaling of various algorithms:

$$\begin{array}{lllll} \textit{implicit}: & E & \propto N^{0} & \propto P^{0} & \propto (1/h)^{0} \\ \textit{explicit advection}: & E & \propto N^{1/d} & \propto P^{1/d} & \propto (1/h) \\ \textit{explicit diffusion}: & E & \propto N^{2/d} & \propto P^{2/d} & \propto (1/h)^{2} \end{array}$$



Expected execution time vs unknowns (procs)



Expected execution time vs resolution

[Keyes, R. & Woodward, 2006]

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Case Study – Magnetic Fusion

Resistive MHD provides the simplest fluid description of fusion plasmas. The model couples the viscous, compressible Euler eqns (fluid flow – $\rho, \rho\mathbf{v}, e$) with the low-frequency Maxwell equations (electromagnetic fields – $\mathbf{B}$):

$$\begin{aligned}
\partial_t \rho + \nabla \cdot (\rho \mathbf{v}) &= 0, \\
\partial_t (\rho \mathbf{v}) + \nabla \cdot \left(\rho \mathbf{v}\mathbf{v}^T - \mathbf{B}\mathbf{B}^T + \left(p + \tfrac{1}{2}\mathbf{B}\cdot\mathbf{B}\right)\bar{\mathrm{I}} \right) &= \nabla \cdot \bar{\tau}, \\
\partial_t e + \nabla \cdot \left((e + p + \tfrac{1}{2}\mathbf{B}\cdot\mathbf{B})\mathbf{v} - \mathbf{B}(\mathbf{B}\cdot\mathbf{v}) \right) &= \nabla \cdot (\bar{\tau}\mathbf{v} + \kappa \nabla T) \\
&\quad + \nabla \cdot \left(\eta \left(\tfrac{1}{2}\nabla(\mathbf{B}\cdot\mathbf{B}) - \mathbf{B}(\nabla\mathbf{B})^T \right) \right), \\
\partial_t \mathbf{B} + \nabla \cdot \left(\mathbf{v}\mathbf{B}^T - \mathbf{B}\mathbf{v}^T \right) &= \nabla \cdot \left(\eta \nabla \mathbf{B} - \eta \left(\nabla \mathbf{B} \right)^T \right).
\end{aligned}$$

Here $e = \frac{p}{\gamma - 1} + \rho \frac{\mathbf{v}\cdot\mathbf{v}}{2} + \frac{\mathbf{B}\cdot\mathbf{B}}{2}$, $T = \frac{p}{\rho\, r_{\text{gas}}}$, and $\bar{\tau} = \mu \left(\nabla\mathbf{v} + (\nabla\mathbf{v})^T \right) - \frac{2}{3}\mu(\nabla\cdot\mathbf{v})\bar{\mathrm{I}}$.

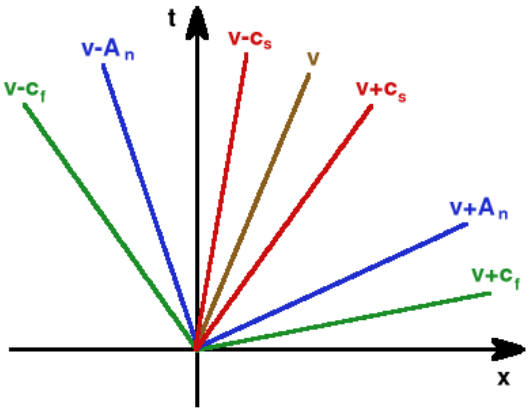
Condensing notation, we rewrite this in terms of $\mathbf{U} = (\rho,\ \rho\mathbf{v},\ \mathbf{B},\ e)^T$:

$$\partial_t \mathbf{U} = -\nabla \cdot \mathbf{F}_h(\mathbf{U}) + \nabla \cdot \mathbf{F}_d(\mathbf{U})$$

Stiffness in Resistive MHD

Resistive MHD stiffness results from fast hyperbolic waves and diffusive effects. The hyperbolic wave speeds are given by

$$\lambda_e = \mathbf{v} \qquad \text{(entropy wave)}$$
$$\lambda_d = \mathbf{v} \qquad \text{(magnetic-flux wave)}$$
$$\lambda_s = \mathbf{v} \pm c_s \qquad \text{(slow magnetosonic)}$$
$$\lambda_a = \mathbf{v} \pm A_n \qquad \text{(Alfvén waves)}$$
$$\lambda_f = \mathbf{v} \pm c_f \qquad \text{(fast magnetosonic)}$$



- For MHD, $c_s \ll A_n < c_f$, and typically $c_f \approx 10^6$.
- Moreover, diffusive (resistive, viscous) effects induce stiffness due to the quadratic CFL condition $\Delta t \propto \Delta x^2$.

Coupling implicitly and using a standard N-K solver [SUNDIALS], we have

$$J(\mathbf{U}) \;=\; I + \Delta t \frac{\partial}{\partial \mathbf{U}} \left[\nabla \cdot \mathbf{F}_h(\mathbf{U})\right] - \Delta t \frac{\partial}{\partial \mathbf{U}} \left[\nabla \cdot \mathbf{F}_d(\mathbf{U})\right] \;=\; I + \Delta t J_h - \Delta t J_d.$$

SUNDIALS: http://www.llnl.gov/casc/sundials/

MHD Preconditioning

We employ an operator-splitting strategy for preconditioning, and set

$$P \;=\; P_h P_d \;=\; [I + \Delta t J_h]\,[I - \Delta t J_d] \;=\; J + \mathcal{O}(\Delta t^2).$$

- P_h solves for the stiff wave effects within the hyperbolic subsystem.
  - 8 coupled linear advection equations,

$$v + \Delta t\,[A\partial_x v + B\partial_y v + C\partial_z v] = b.$$

  - Split by direction and then decompose along characteristics.
  - Solved using parallel tridiagonal solvers on structured spatial grids.
- P_d solves the remaining diffusive effects.
  - 3 decoupled "heat-like" equations (1 scalar, 2 vector),

$$(I - \Delta t \nabla^2) w = c.$$

  - Solved using optimal geometric multigrid methods [HYPRE].

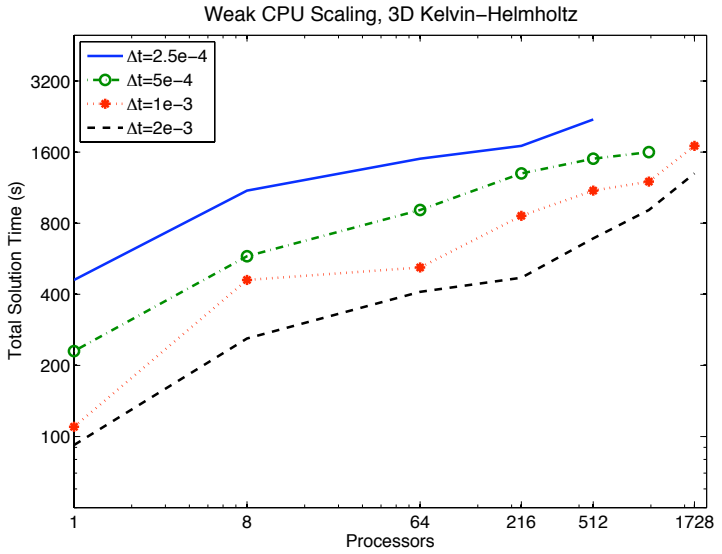
P_h: [R., Samtaney & Woodward, 2008]
Combined P: [R., Samtaney & Woodward, *in prep.*]

HYPRE: http://www.llnl.gov/casc/hypre/

MHD Preconditioner Results

Δx	Method	CPU Time	Nt
0.4	Exp	75 s.	1636
0.2	Exp	768 s.	3247
0.1	Exp	8214 s.	6493
0.05	Exp	80348 s.	12985
0.4	Imp	47 s.	1144
0.2	Imp	285 s.	1158
0.1	Imp	1817 s.	1075
0.05	Imp	14203 s.	1473

Explicit/Implicit time ratios: 1.6, 2.7, 4.5, 5.7

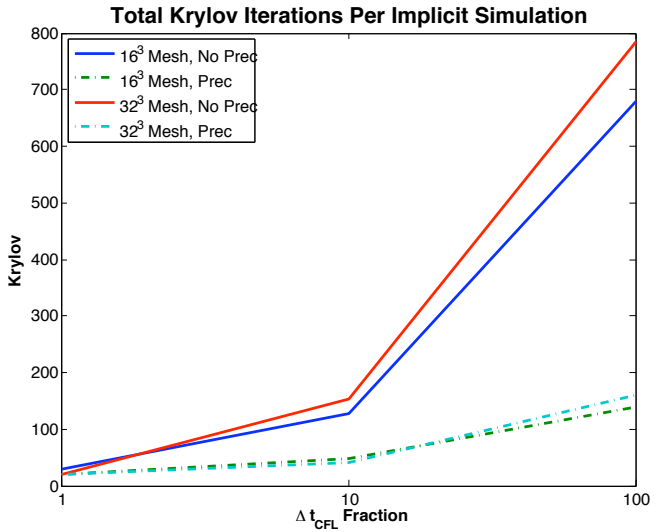


Explicit vs implicit (no P) timings on Magnetic Reconnection problem (above),

Weak CPU scaling using P_h preconditioner: Kelvin Helmholtz test (corner),

Linear iterations using P_d preconditioner: diffusion-dominated test (right).

[scaling tests run on LLNL *Thunder* cluster]



Case Study – Cosmic Reionization

We consider the cosmological radiation-hydrodynamics-chemistry system,

$$\partial_t \rho_b + \frac{1}{a}\mathbf{v}_b \cdot \nabla \rho_b = -\frac{1}{a}\rho_b \nabla \cdot \mathbf{v}_b,$$

$$\partial_t \mathbf{v}_b + \frac{1}{a}(\mathbf{v}_b \cdot \nabla)\mathbf{v}_b = -\frac{\dot{a}}{a}\mathbf{v}_b - \frac{1}{a\rho_b}\nabla p - \frac{1}{a}\nabla\phi,$$

$$\partial_t e + \frac{1}{a}\mathbf{v}_b \cdot \nabla e = -\frac{2\dot{a}}{a}e - \frac{1}{a\rho_b}\nabla \cdot (p\mathbf{v}_b) - \frac{1}{a}\mathbf{v}_b \cdot \nabla\phi + G - \Lambda,$$

$$\partial_t \mathbf{n}_i + \nabla \cdot (\mathbf{n}_i \mathbf{v}_b) = -3\frac{\dot{a}}{a}\mathbf{n}_i - \mathbf{n}_i \Gamma_i^{ph} + \alpha_{i,j}^{rec}\mathbf{n}_e \mathbf{n}_j,$$

$$\partial_t E + \frac{1}{a}\nabla \cdot (E\mathbf{v}_b) - \frac{1}{a^2}\nabla \cdot (D\,\nabla E) = -4\frac{\dot{a}}{a}E + 4\pi\eta - ckE,$$

$$\nabla^2 \phi = -\frac{4\pi G}{a}\rho_b,$$

coupling hydrodynamics $(\rho, \mathbf{v}_b, e)$, species number densities $(\mathbf{n}_i)$, grey radiation energy density (E), and gravitational potential (ϕ). G and Λ correspond to energy sources and sinks due to radiation and chemical couplings.

$a(t) = \frac{1}{1+z}$ provides cosmological expansion, $\mathbf{x} = \frac{\mathbf{r}}{a(t)}$ is the comoving distance.

Operator Split Multi-physics Approach – I

We wish to add radiation-chemistry physics to ENZO, an optimized code for AMR hydrodynamics and self-gravity. Decomposing $e = e_h + e_c$, we have

$$\partial_t(e_h + e_c) + \frac{1}{a}\mathbf{v}_b \cdot \nabla e = -\frac{2\dot{a}}{a}(e_h + e_c) - \frac{1}{a\rho_b}\nabla \cdot (p\mathbf{v}_b) - \frac{1}{a}\mathbf{v}_b \cdot \nabla\phi + G - \Lambda.$$

In operator-split fashion, Enzo explicitly evolves one time step of the system:

$$\partial_t \rho_b + \frac{1}{a}\mathbf{v}_b \cdot \nabla \rho_b = -\frac{1}{a}\rho_b \nabla \cdot \mathbf{v}_b,$$

$$\partial_t \mathbf{v}_b + \frac{1}{a}(\mathbf{v}_b \cdot \nabla)\mathbf{v}_b = -\frac{\dot{a}}{a}\mathbf{v}_b - \frac{1}{a\rho_b}\nabla p - \frac{1}{a}\nabla\phi,$$

$$\partial_t e_h + \frac{1}{a}\mathbf{v}_b \cdot \nabla e_h = -\frac{2\dot{a}}{a}e_h - \frac{1}{a\rho_b}\nabla \cdot (p\mathbf{v}_b) - \frac{1}{a}\mathbf{v}_b \cdot \nabla\phi,$$

$$\partial_t \mathbf{n}_i + \nabla \cdot (\mathbf{n}_i \mathbf{v}_b) = 0,$$

$$\partial_t E + \frac{1}{a}\nabla \cdot (E\mathbf{v}_b) = 0,$$

$$\nabla^2 \phi = -\frac{4\pi G}{a}\rho_b.$$

Operator Split Multi-physics Approach – II

We then tackle the remainder of the original system with an implicit approach,

$$\partial_t e_c = -2\frac{\dot{a}}{a}e_c + G - \Lambda,$$

$$\partial_t \mathtt{n}_i = -3\frac{\dot{a}}{a}\mathtt{n}_i - \mathtt{n}_i\Gamma_i^{ph} + \alpha_{i,j}^{rec}\mathtt{n}_e\mathtt{n}_j, \quad (i,j=1,\ldots,n_s)$$

$$\partial_t E = \frac{1}{a^2}\nabla\cdot(D\,\nabla E) - 4\frac{\dot{a}}{a}E + 4\pi\eta - ckE.$$

An implicit discretization of this system results in a Jacobian of the form

$$J = I + \Delta t \begin{bmatrix} J_{e,e} & J_{e,\mathtt{n}} & J_{e,E} \\ J_{\mathtt{n},e} & J_{\mathtt{n},\mathtt{n}} & J_{\mathtt{n},E} \\ J_{E,e} & J_{E,\mathtt{n}} & J_{E,E} \end{bmatrix},$$

in which all blocks are spatially-local except for $J_{E,E}$, which contains the term

$$-\frac{\partial}{\partial E}\left[\nabla\cdot(D\,\nabla E)\right].$$

Schur-Krylov-MG Linear Solver

Combining variables $x_M = (x_e, x_\mathbf{n})$ we write $Jx = b$ as

$$\begin{bmatrix} M & U \\ L & D \end{bmatrix} \begin{pmatrix} x_M \\ x_E \end{pmatrix} = \begin{pmatrix} b_M \\ b_E \end{pmatrix}.$$

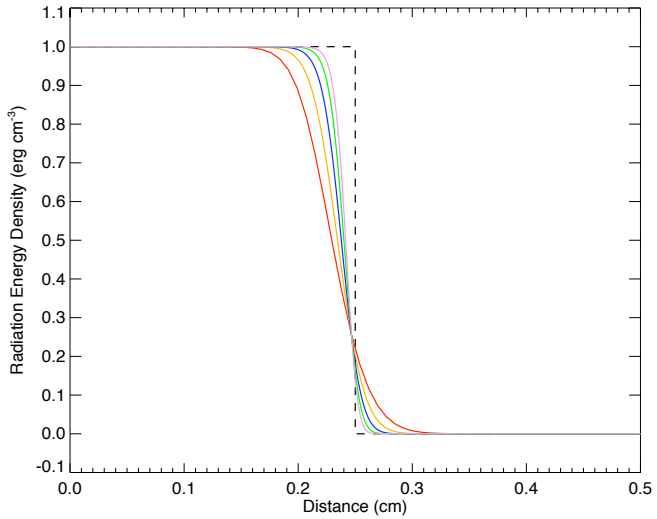
Since M^{-1} is simple to compute (block-diagonal), we use a Schur complement formulation to solve for x,

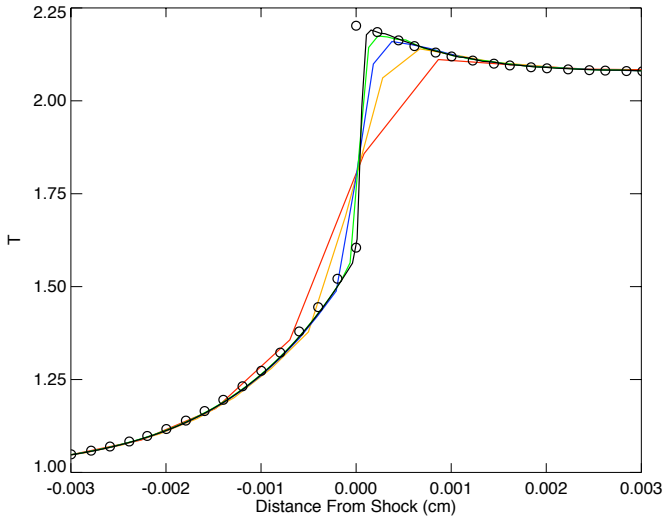
$$Mx_M + Ux_E = b_M \quad \Rightarrow \quad x_M = M^{-1}(b_M - Ux_E),$$
$$(D - LM^{-1}U)x_E = b_E - LM^{-1}b_M.$$

Implementation notes:

- The "heat-like" system $(D - LM^{-1}U)x_E = b_E - LM^{-1}b_M$ is solved with a Conjugate Gradient iteration.
- The CG solver is preconditioned with geometric multigrid [HYPRE].
- x_M is then easily computed from x_E.

Cosmology Results



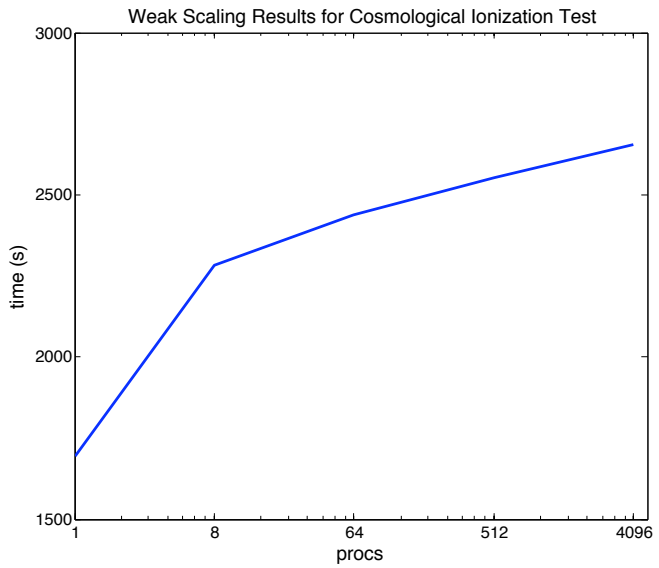


Solution convergence on streaming radiation test (top),

Solution convergence on radiating shock test due to Lowrie & Edwards (corner),

Weak CPU scaling on a cosmological ionization problem due to Shapiro & Giroux (right).

[scaling tests run on NSF/NICS *Kraken* machine]



Conclusions

- Multi-physics couplings may be achieved in a variety of ways:
  - Explicit, Time-subcycled, Mixed IMEX, Fully Implicit.
  - Decision depends on stiffness & separability of system.
  - Coupling method will dictate stability, accuracy, and scalability limitations of the overall simulation.
- Implicitly-coupled formulations promise scalability, stability and accuracy, but at a cost:
  - Large-scale nonlinear solvers become a necessity.
  - There is a well-documented approach (Newton-Krylov), available through a number of highly configurable and effective solver libraries.
  - True robustness and scalability for real-world problems may require application-specific knowledge in the preconditioner.

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Newton Robustness Improvements

Newton robustness w.r.t. initial guess is often accomplished with globalization methods: attempt to generate iterates within Newton convergence radius:

- *Line search*: adjusts Newton update to increase Newton radius of convergence.
- *Begin with another method*: use a slower, more globally-convergent method (e.g. Picard iteration) at first to obtain initial Newton iterate.
- *Improved initial guess*: use another method to generate a better initial Newton iterate (e.g. explicit predictor for time-dependent problems).
- *Trust region*: combines Newton direction with steepest-descent direction to ensure initial convergence.
- *Continuation*: iterative solver using Newton method for problems involving bifurcations, phase transitions or steady-state calculations.