Selected Topics in Accelerator Theory and Simulation

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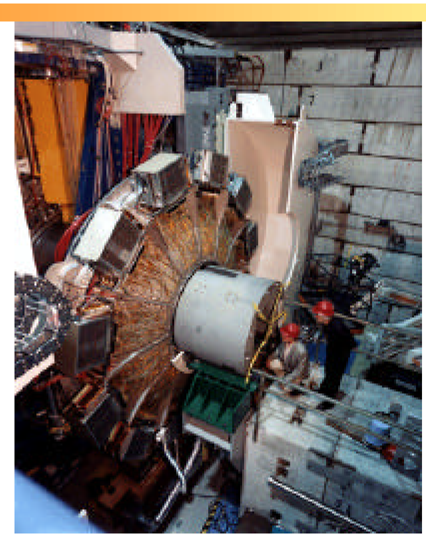
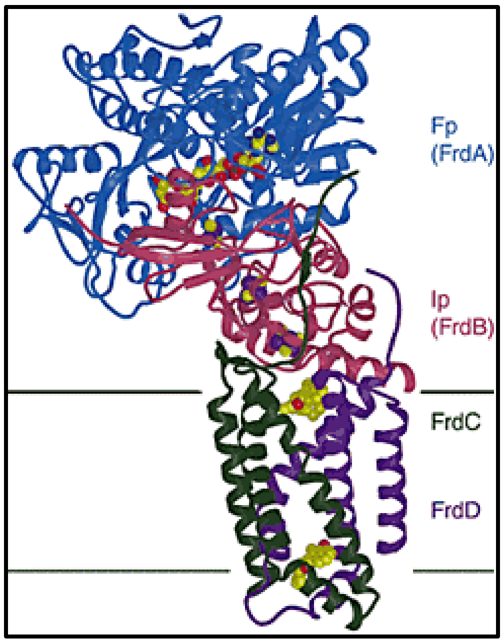
- Part I: Particle accelerator overview
- Part II: High performance computing in accelerator physics
- Part III: Symplectic methods in accelerator physics
- Part IV: Symplectic methods for infinite-dimensional systems

Accelerators are Crucial to Scientific Discoveries in Particle Physics, Materials Science, Chemistry, and Biological Science

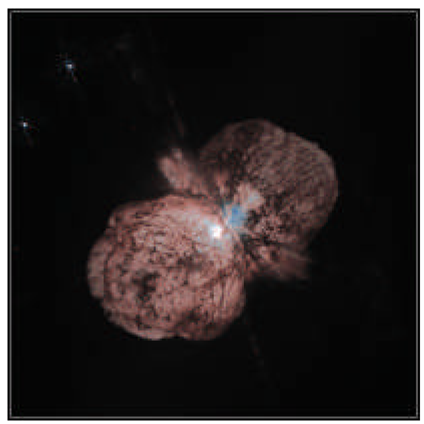
- Accelerators for high energy physics
- Accelerators for nuclear physics
- Synchrotron light sources
- Spallation neutron sources



"Violated particles reveal quirks of antimatter"



"Biologists and other researchers are lining up at synchrotrons to probe materials and molecules with hard x-rays"



"A new generation of accelerators capable of generating beams of exotic radioactive nuclei aims to simulate the element-building process in stars and shed light on nuclear structure"

The Advanced Light Source (ALS) at Lawrence Berkeley National Laboratory.

CERN site showing LEP (Large Electron Positron Collider), the largest accelerator in the world. Future site of the Large Hadron Collider (LHC)

Accelerator Components

- Examples of beamline elements
  - rf cavities (acceleration)
  - magnetic dipole (bending)
  - magnetic quadrupole* (transverse focusing)
  - magnetic multipoles: sextupole, octupole,…
    (influences nonlinear behavior)

Sextupole

Quadrupole

- A sequence of beamline elements = a *beamline* or *lattice*

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*A single quad *does not* focus both transverse directions simultaneously

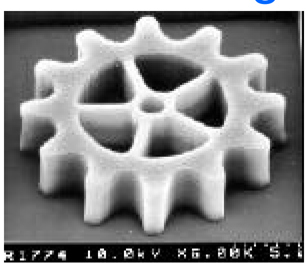
– an x-focusing quad is y-defocusing (and vice-versa)

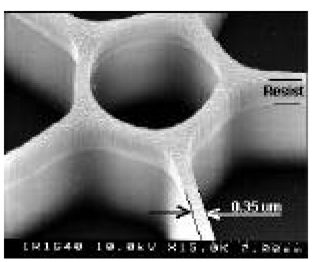
– a sequence of quads of opposite polarity *can* focus in both planes (just as a sequence of convex/concave lenses may guide light)

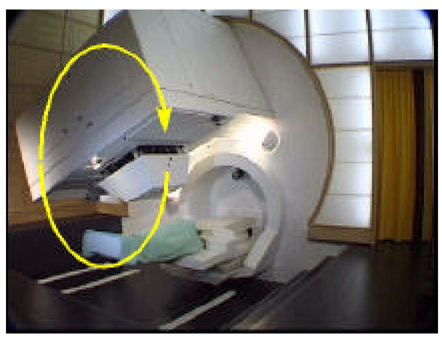
– example: “FODO” lattice = x-focus,drift,x-defocus,drift,...

Contributions of accelerators have significant economic impact and greatly benefit society

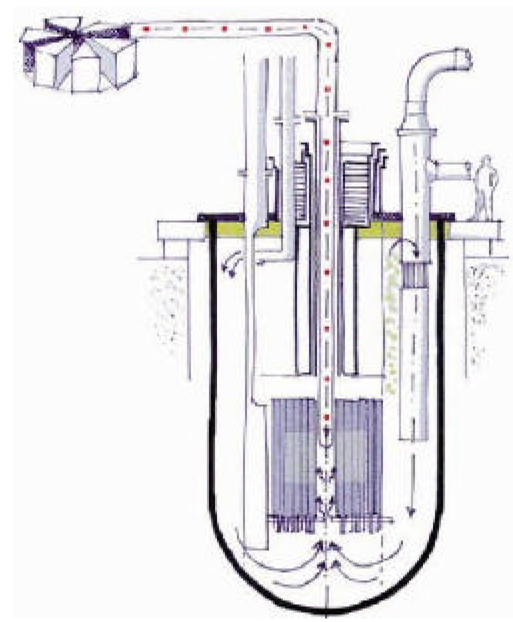
- Medical isotope production
- Electron microscopy
- Accelerator mass spectrometry
- Medical irradiation therapy
- Ion implantation
- Beam lithography





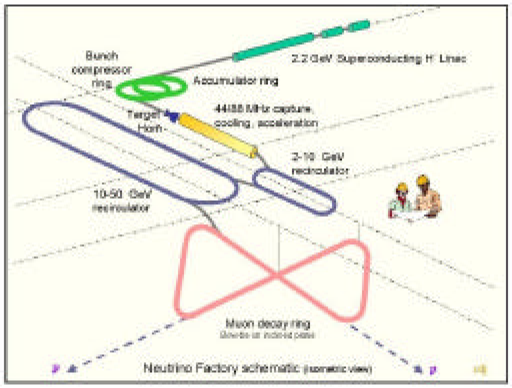


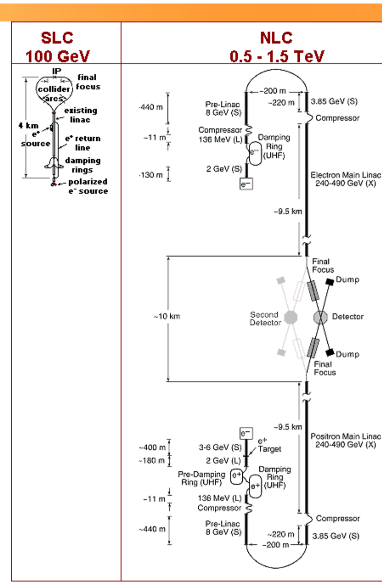
- Transmutation of waste
- Accelerator-driven energy production
- Hydrodynamic imaging



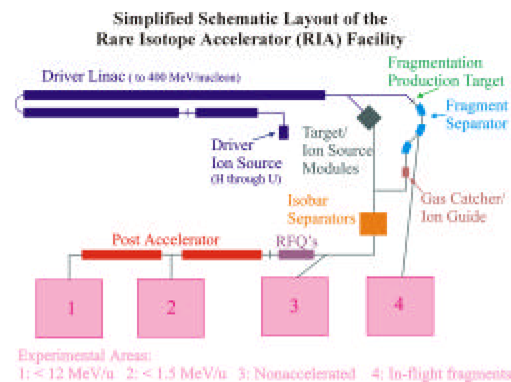
Opportunities at Next-Generation Accelerator Facilities

Exploring physics beyond the Standard Model. Are there new particles? New interactions?

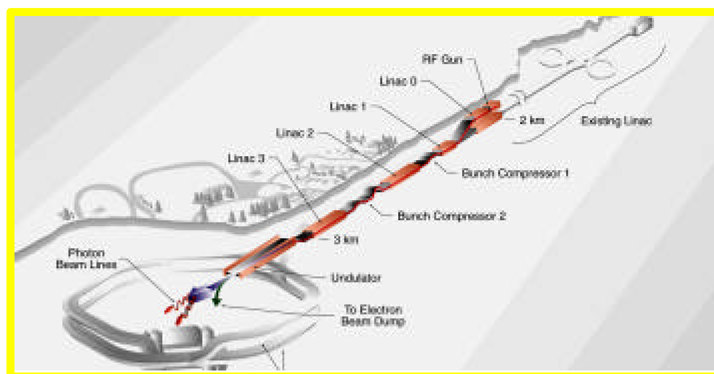




Research with exotic nuclei:
The nature of nucleonic matter; origin of the elements; tests of the Standard Model

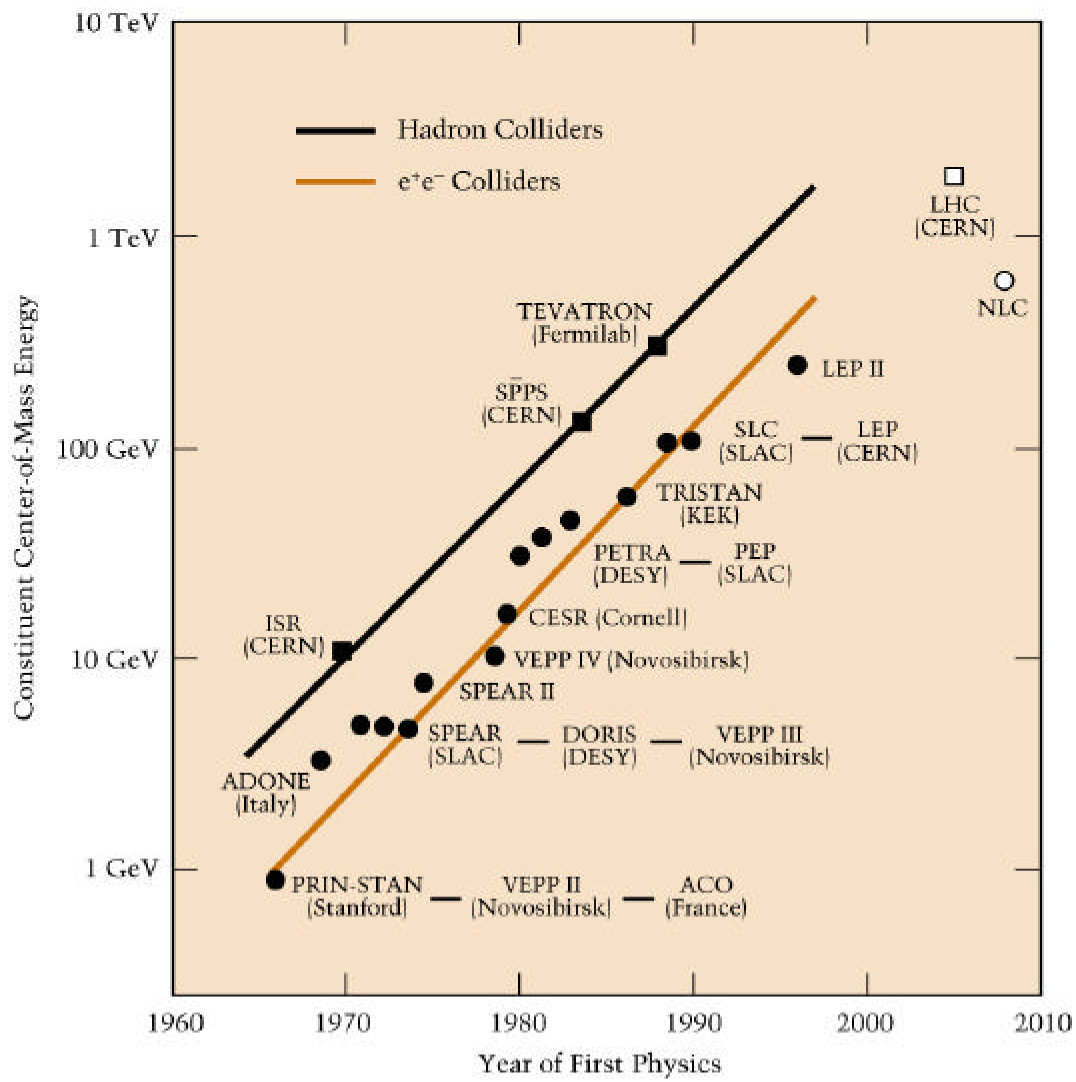


Research using intense, ultra-short pulses of x-ray radiation (4th generation light source): fundamental quantum mechanics; atomic, molecular, and optical physics; chemistry; materials science; biology



Issues for Next-Generation Accelerators

- Cost of leading-edge accelerators: several billion $
- Design decisions can have huge consequences
  - Supercollider example:
    beam pipe aperture change from 3cm to 4cm cost est. $1B
- Existing technology facing barriers
  - **Falling off "Livingston Curve"**



Panofsky and Breidenbach,
Rev. Mod. Phys. 71, #2 (1999)

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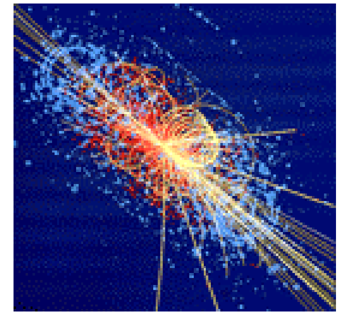
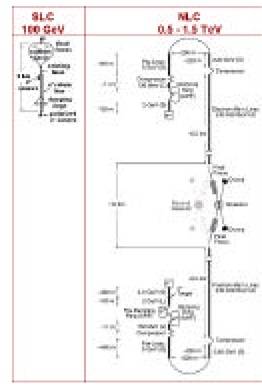
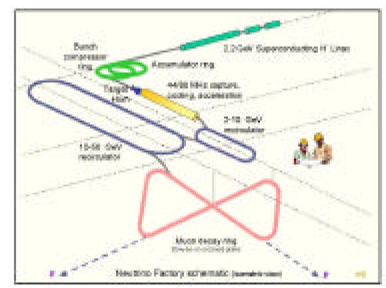
High Performance Computing is Playing a Major Role in Accelerator Science & Technology

- Present accelerators: Maximize investment by
  - optimizing performance
  - expanding operational envelopes
  - increasing reliability and availability

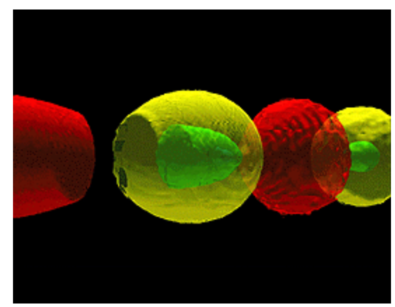




- Next-generation accelerators
  - better designs
  - feasibility studies
  - Facilitate important design decisions
  - completion on schedule and within budget



- Accelerator science and technology
  - help develop new methods of acceleration
  - explore beams under extreme conditions



Parallel Code Development

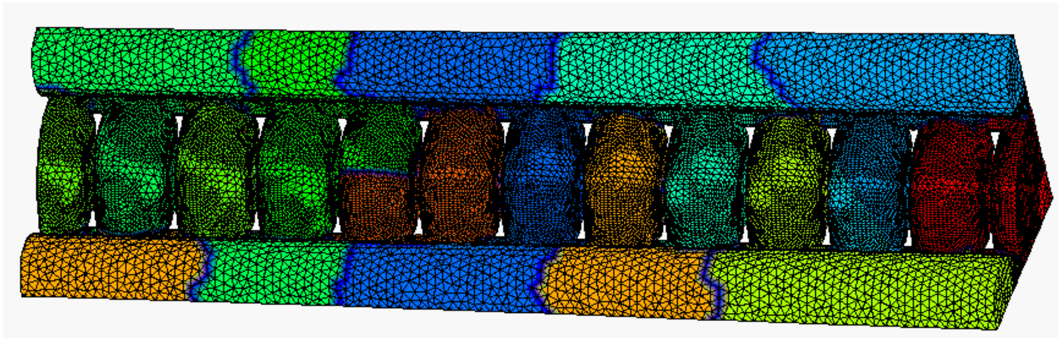
- Electromagnetics (EM)

  Maxwell's equations
  - Eigenmode
  - Time-domain
  - Statics
- Beam Dynamics

  Hamilton; Vlasov/Poisson
  - High intensity beams in linacs & rings
- Coupled EM/beams

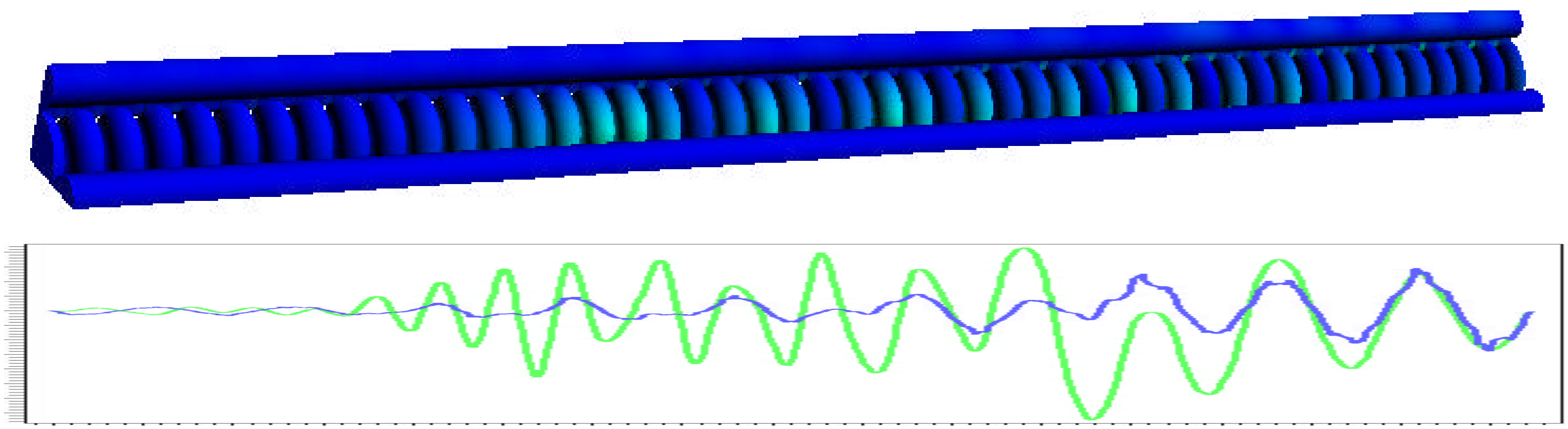
  Vlasov/Maxwell
  - Laser/Plasma-based accelerators

SLAC is developing a parallel eigensolver: *Omega3P*



12 cell stack

Calculation of modes in entire structure has begun

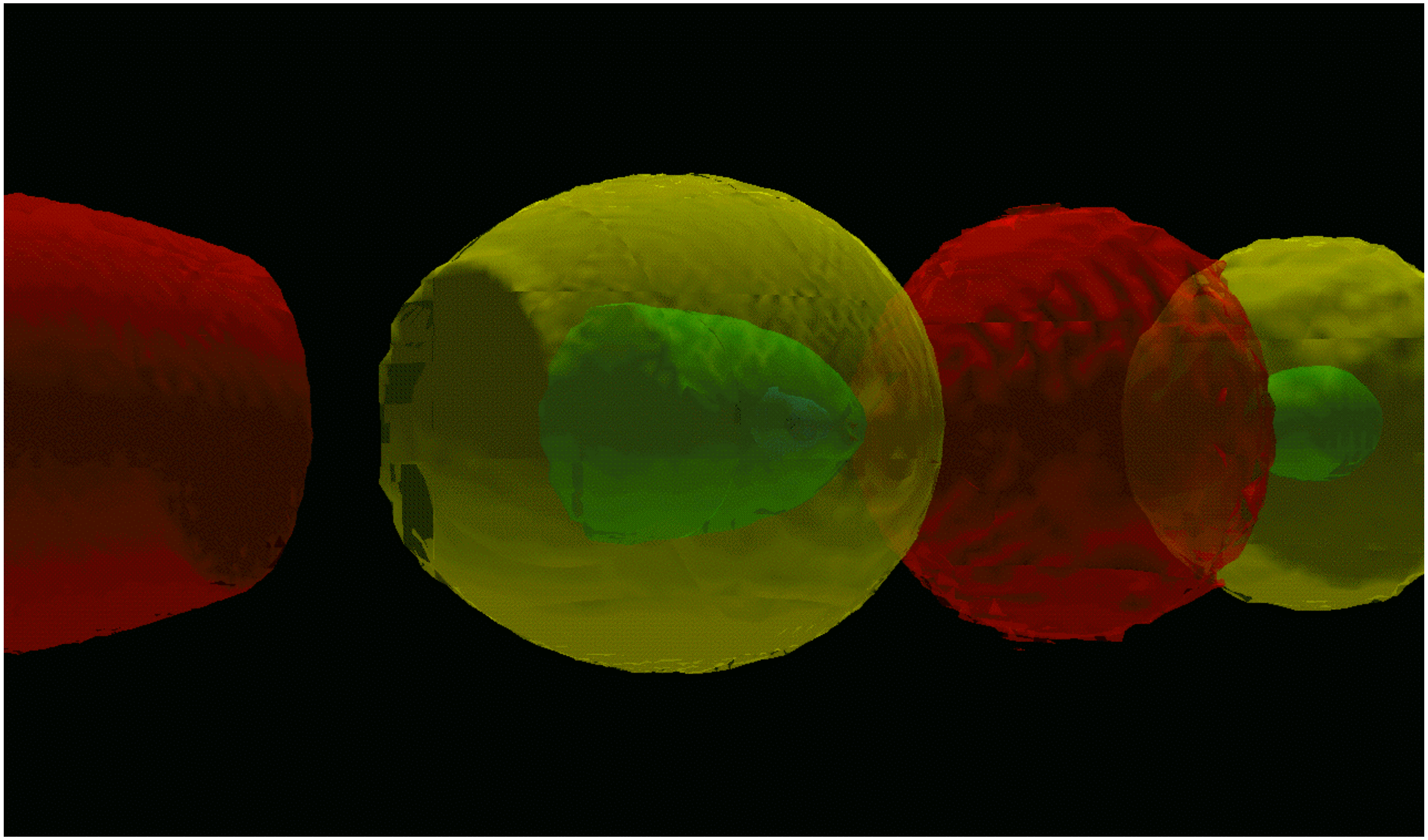


Cavity field

Manifold field

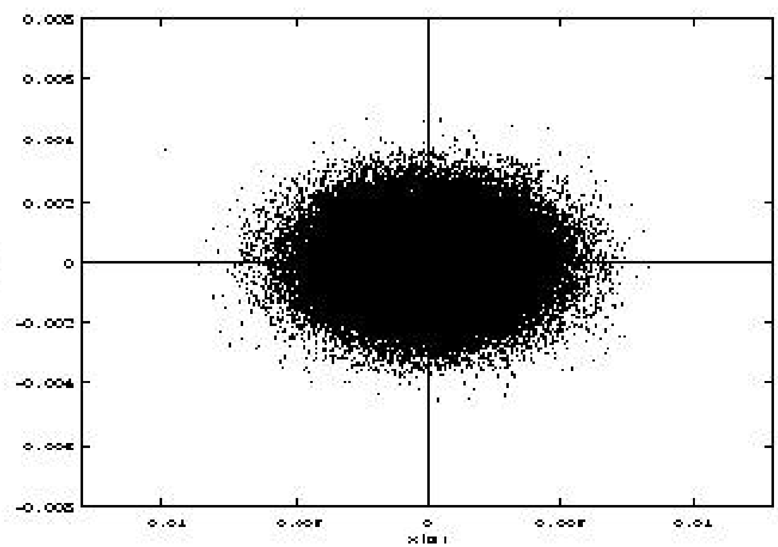
Plasma Wakefield Accelerator

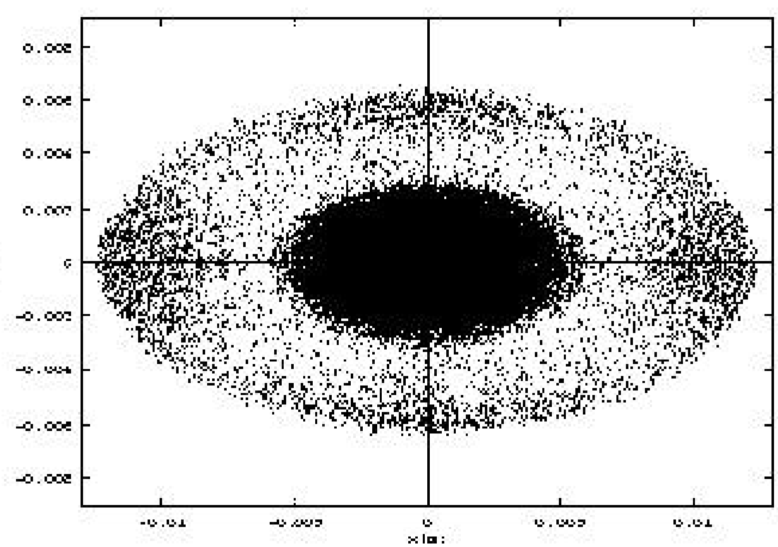
Isosurface contours of the accelerating structure in a PWFA



High Intensity Beam Dynamics

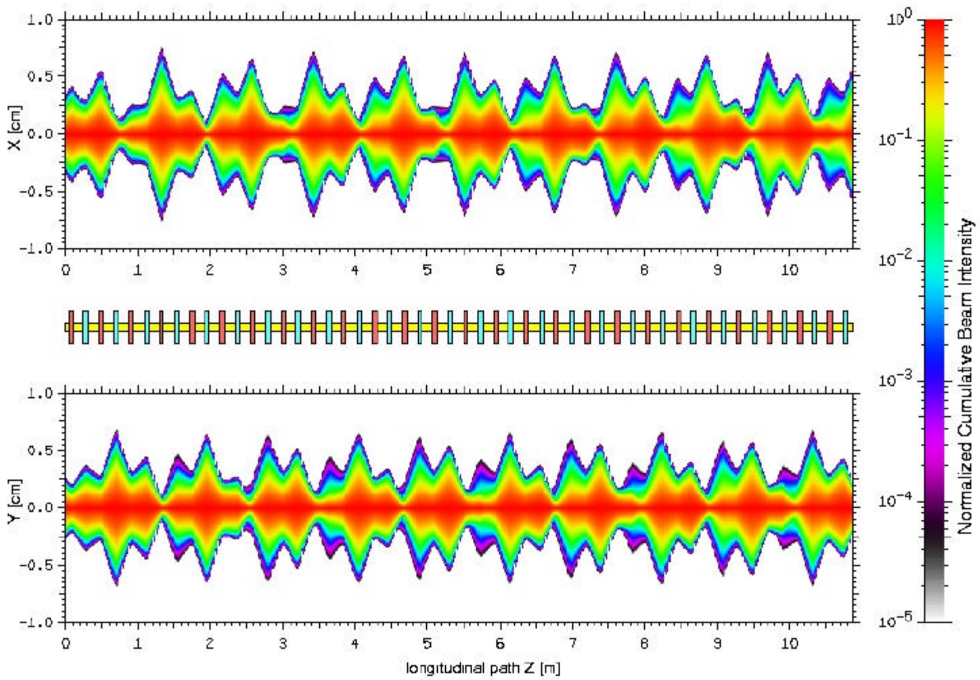
- Beam losses are a key issue for accelerators operating at the high-intensity frontier
  - Fermilab booster, Brookhaven AGS, SNS accumulator
  - Future proton drivers for neutrino factories, muon colliders
- Need to understand, control beam halos



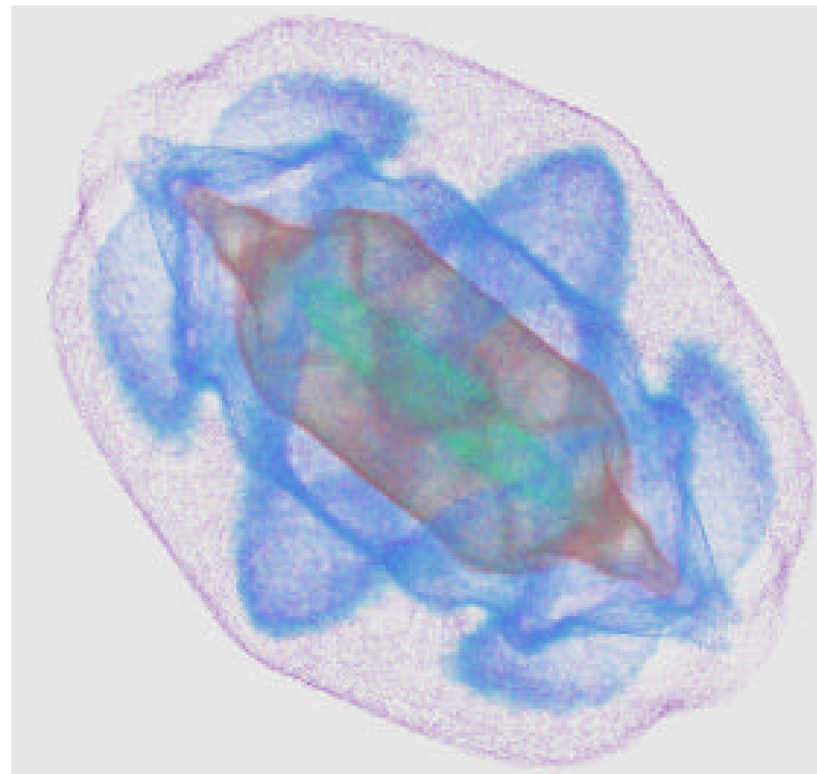


Beam Dynamics: Old vs. New Capability

- 1980s: 10K particle, 2D serial simulations
- Early 1990s: 10K-100K, 2D serial simulations
- 2000: 100M (5-10 hrs on 256 PEs);
  more realistic models



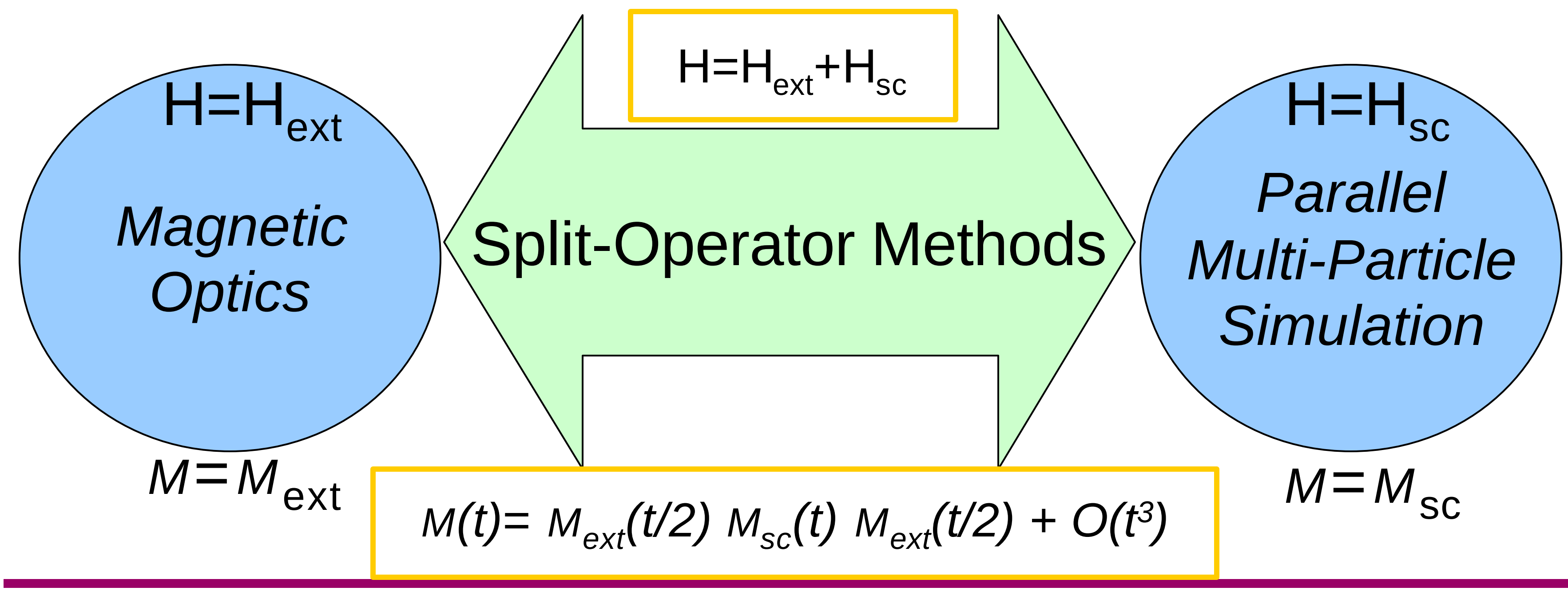
LEDA halo expt; 100M particles



Visualization of beam distribution function in phase space

We are using Split-Operator Methods to Develop Parallel Codes to Model High Intensity Beams

- 3D Parallel Particle-In-Cell Code to solve the Vlasov/Poisson equations
- Philosophy:
  - Do not take tiny steps to push ~100M particles
  - Do take tiny steps to compute transfer maps; then push w/ maps



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Hamiltonian description of charged particle dynamics in electromagnetic fields

- Cartesian w/ t as the independent variable:

$$H(x, p_x, y, p_y, z, p_z; t) = \sqrt{m^2c^4 + c^2(\vec{p} - q\vec{A})^2} + q\Phi$$

- Cartesian w/ z as the independent variable:

$$K(x, p_x, y, p_y, t, p_t; z) =$$

$$-\sqrt{(p_t + q\Phi)^2 / c^2 - m^2c^2 - (p_x - qA_x)^2 - (p_y - qA_y)^2} - qA_z$$

- Usually this is expanded about a *reference trajectory*
  - perturbation theory performed for small deviations around the reference trajectory
  - results in Hamiltonians w/ 10s, 100s, or 1000s of terms

Hamiltonian dynamics, cont.

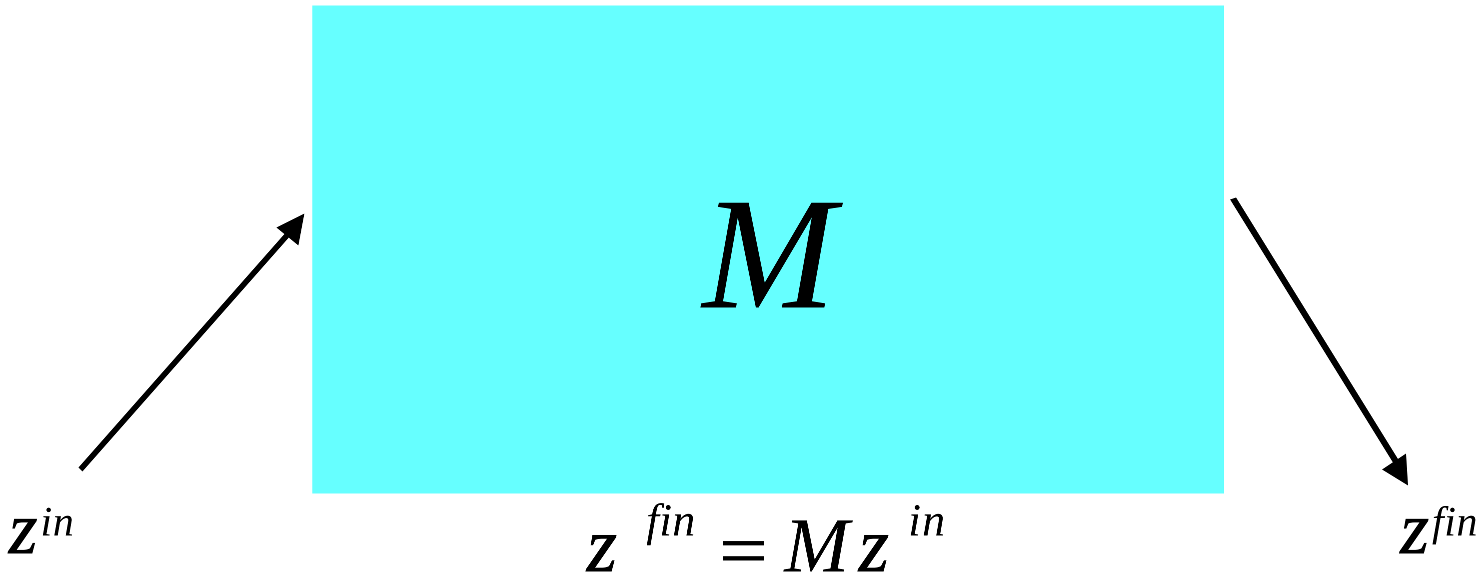
- Different beamline elements have different potentials
- Example: a quadrupole w/ gradient g(z):

$$A_x = \frac{1}{4} g'(z)(x^3 - xy^2) + \dots$$

$$A_y = \frac{1}{4} g'(z)(x^2 y - y^3) + \dots$$

$$A_z = \frac{g(z)}{2}(y^2 - x^2) - \frac{1}{12} g''(z)(y^4 - x^4) + \dots$$

Transfer Maps



$$z^{fin} = Mz^{in}$$

$z = (x, p_x, y, p_y, z, p_z)$

Lie Operators and Lie Transformations

$$[f,g] = \sum_{i=1}^{3}\left(\frac{\partial f}{\partial x_i}\frac{\partial g}{\partial p_i} - \frac{\partial f}{\partial p_i}\frac{\partial g}{\partial x_i}\right) \equiv :f:g$$

Lie Operator

$$:f:^0 g = g$$

$$:f:^1 g = [f,g]$$

$$:f:^2 g = [f,[f,g]]$$

$$\ldots$$

Note well: If P_n is a homogenous polynomial of degree n, then, when its associated Lie operator is applied to a phase space variable, $:P_n:z_a$ is of degree n-1

Lie Transformation:

$$e^{:f:}g = g + :f:g + \frac{1}{2}:f:^2 g + \ldots$$

Symplectic Mappings

- Hamilton's equations:

$$\frac{dV}{dt} = -:H:V$$

- Formal solution (time-independent case):

$$M = \mathrm{e}^{-t:H:}$$

- Lie transformations are symplectic mappings. They provide a natural and powerful formalism to describe, parameterize, and manipulate symplectic maps.

Representation of Transfer Maps

Taylor Series:

$$z_a^{fin} = \sum_{b=1}^{6} R_{ab} z_b^{in} + \sum_{b,c=1}^{6} T_{abc} z_b^{in} z_c^{in} + \sum_{b,c,d=1}^{6} U_{abcd} z_b^{in} z_c^{in} z_d^{in} + \ldots$$

Lie Representation: (Dragt & Finn)

$$M = e^{:f_2:} e^{:f_3:} e^{:f_4:} \ldots$$

where f_n is a homogeneous polynomial of degree n

Comparison of the Methods

$$z_a^{fin} = \sum_{b=1}^{6} R_{ab} z_b^{in} + \sum_{b,c=1}^{6} T_{abc} z_b^{in} z_c^{in} + \sum_{b,c,d=1}^{6} U_{abcd} z_b^{in} z_c^{in} z_d^{in} + \ldots$$

$$M = e^{:f_2:} e^{:f_3:} e^{:f_4:} \ldots$$

$$= e^{:f_2:}(1 + :f_3: + + \frac{1}{2} f_3^2 \ldots)(1 + :f_4: + \ldots)(\ldots)$$

$$Mz = e^{:f_2:} z + e^{:f_2:} :f_3: z + e^{:f_2:}(:f_4: + \frac{1}{2} f_3^2 + \ldots) z + \ldots$$

Lie Polynomials

1 x 2 p_x 3 y 4 p_y 5 t 6 p_t	*1st order monomials: displacements*	28 x^3 29 x^2p_x 30 x^2y 31 x^2p_y … … 82 p_t^2t 83 p_t^3	*3^{rd} order monomials: lowest order aberrations (sextupoles,…)*
7 x^2 8 xp_x 9 xy 10 xp_y … … 26 tp_t 27 p_t^2	*2nd order monomials: linear dynamics (paraxial ray optics)*	84 x^4 85 x^3p_x 86 x^3y 87 x^3p_y … … 208 p_t^3t 209 p_t^4	*4^{th} order monomials: octupoles,repeated sextupoles,…*

Lie Methods have Revolutionized the Design and Analysis of Particle Accelerators

- Introduced by Alex Dragt ~ 1980
  - Early response from accelerator community was: fancy mathematics, too complicated
  - Now seen as an indispensable tool for high order optical design
  - Normal form techniques of Dragt and Forest essential for analysis of circular machines
- Related developments
  - Automatic differentiation techniques (Berz) – enables computations of arbitrarily high order maps
  - Symplectic integration techniques
    - Ruth, Forest, Yoshida, Suzuki, Laskar,…

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If we are interested in long-term behavior in a Hamiltonian system (particle in an accelerator, gravitationally interacting system of masses,…) no modern dynamicist would write down equations of motion,

$$\frac{dx}{dt} = v, \quad \frac{dv}{dt} = F/m$$

and develop an integrator by inspection based on:

$$\boxed{\frac{x_{n+1} - x_n}{\Delta t} = v_{n+1/2}} \qquad \boxed{\frac{v_{n+1/2} - v_{n-1/2}}{\Delta t} = F_n / m}$$

- OK for illustrative purposes
- What if the force is a complicated function of x,v?
- What if we are interested in high order, high accuracy integration?

Philosophy

- The development of symplectic algorithms for Hamiltonian systems focuses on the Hamiltonian/Lagrangian or evolution operator.

We should not attempt to develop algorithms for Hamiltonian systems by focusing on the equations of motion

- *But this is exactly how the most widely used method for solving Maxwell's equations (FDTD) has been developed!*

Symplectic Discretizations for Maxwell's Equations

- Involves discretization of the Hamiltonian density

$$H(A,E)=\frac{1}{2}\int\left(\left|\nabla\times A\right|^2+\left|E\right|^2-2J\bullet A\right)dx \qquad (\mu=\varepsilon=1)$$

- Previous work by Xiaowu Lu and Rudolf Schmid, "Symplectic Discretizations for Maxwell's Equations," from the Int'l Conf. On New Applications of Multisymplectic Field Theories, Salamanca, Spain, Sept. 1999. See also http://www.mathcs.emory.edu/~rudolf
  - Proposes an alternative to the usual approach of discretization in space followed by time-integration using a symplectic integrator.

Recent work of Kole, Figge, and De Raedt (Phys. Rev. E. 64, 0667045, Nov 2001)

Expresses Maxwell's equations as

$$\frac{\partial}{\partial t}\Psi(t) = H\,\Psi(t)$$

where H is skew symmetric and $\Psi=(\mu^{1/2}\mathbf{H}(t),\varepsilon^{1/2}\mathbf{E}(t))$. Hence

$$\Psi(t) = e^{tH}\,\Psi(0)$$

where $U(t)=e^{tH}$ is orthogonal.

In this approach, the discretized matrix H is separated into skew symmetric parts H_e+H_o so that e^{He} and e^{Ho} are also orthogonal. Then a Suzuki/Yoshida product is used to approximate U(t). Therefore the evolution operator is a product of orthogonal matrices, and is unconditionally stable.

Example: 1D Wave Equation $\frac{\partial^2 u}{\partial t^2} = v^2 \frac{\partial^2 u}{\partial x^2}$

- Kole/Figge/De Raedt approach: Dynamical variables are X and Y, where

$$\frac{\partial X}{\partial t} = v\frac{\partial Y}{\partial x} \qquad \frac{\partial Y}{\partial t} = v\frac{\partial X}{\partial x}$$

- Spatial derivatives of X and Y are approximated by finite differences on interleaved grids, then Ψ=(X,Y) is shown to satisfy $\partial\Psi/\partial t = H\,\Psi$, where the matrix *H* is given by [$\beta=1/(v\,\Delta x)$]

$$H = \sum_{odd}\left[b_{i+1,i}(\mathbf{e}_i\mathbf{e}_{i+1}^T - \mathbf{e}_{i+1}\mathbf{e}_i^T) + b_{i+1,i+2}(\mathbf{e}_{i+1}\mathbf{e}_{i+2}^T - \mathbf{e}_{i+2}\mathbf{e}_{i+1}^T)\right]$$

- A product integrator is obtained by writing *H* as a sum of NxN matrices each consisting of 2x2 blocks on the diagonal

Symplectic approach #1: Use finite difference discretization of the the spatial derivatives in the wave equation

$$\frac{\partial^2 u_k}{\partial t^2} = v^2 \frac{u_{k+1} - 2u_k + u_{k+1}}{h^2}$$

- This equation can be derived from the Hamiltonian (v^2=T/m),

$$H = \frac{1}{2m}\sum_k p_k^2 + \frac{T}{2h^2}\sum_k (u_{k+1} - u_k)^2$$

- This also works for a 4th order approximation to $\partial^2/\partial x^2$

Symplectic approach #2: Discretize the Lagrangian Density

$$L = \int \left[\frac{1}{2} r \left(\frac{\partial u}{\partial t} \right)^2 - \frac{1}{2} T \left(\frac{\partial u}{\partial x} \right)^2 \right]$$

- We can discretize using finite element basis functions. The result is that $L = \Sigma L_k$, where, for linear finite elements,

$$L_k = \frac{r}{6}(\dot{u}_k^2 + \dot{u}_k \dot{u}_{k+1} + \dot{u}_{k+1}^2) - \frac{T}{2h^2}(u_{k+1} - u_k)^2$$

- Can also be done for quadratic and higher order elements
- Problem: To obtain the discrete Hamiltonian, we have to obtain the corresponding momenta. This requires solving a sparse linear system whose solution is dense.

Symplectic approach #3: Discretize the Hamiltonian Density

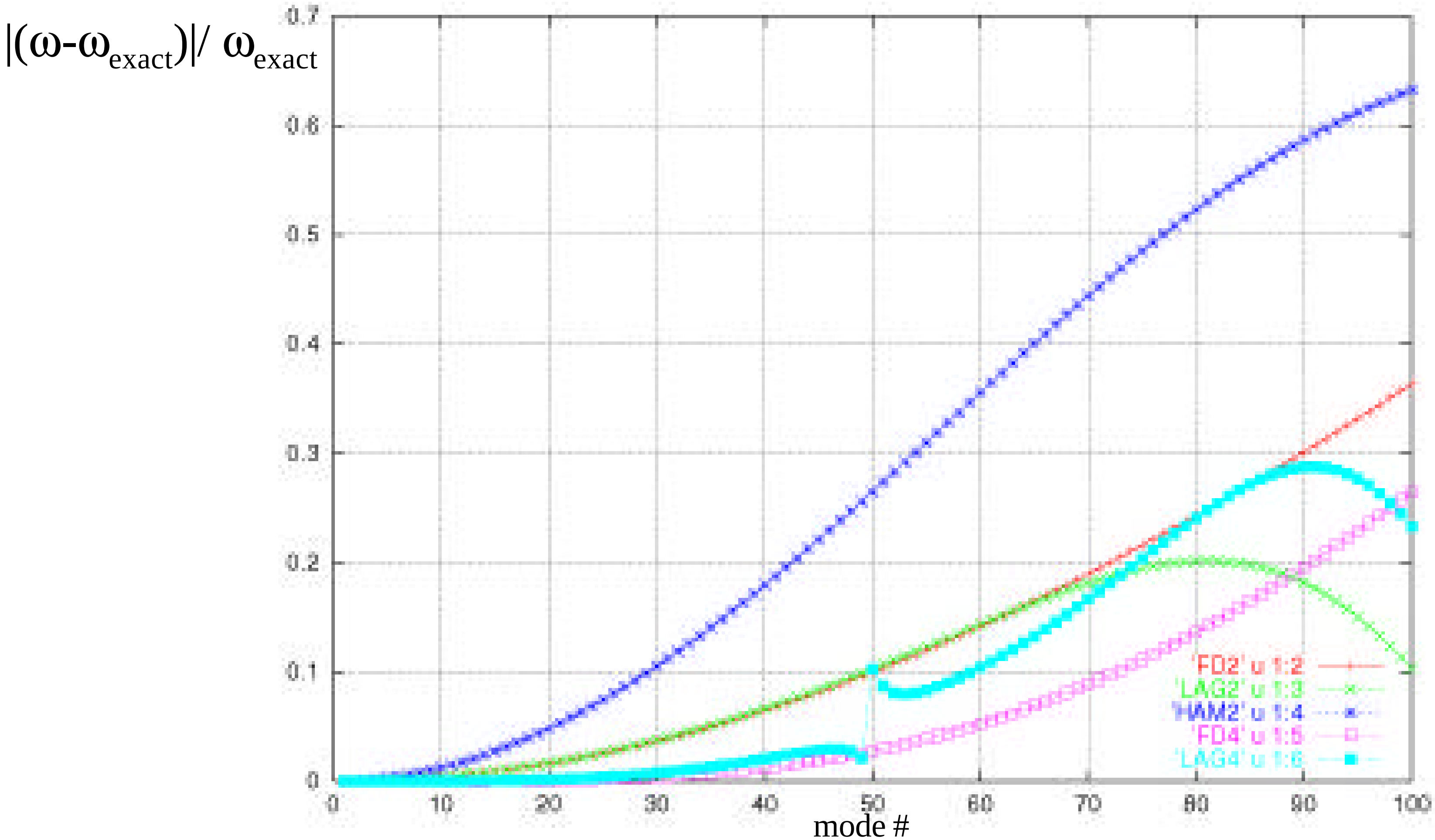
$$H = \int \left[\frac{1}{2r} p^2 + \frac{1}{2} T \left(\frac{\partial u}{\partial x} \right)^2 \right]$$

- We can discretize using finite element basis functions. The result is that $H = \Sigma H_k$, where, for linear finite elements,

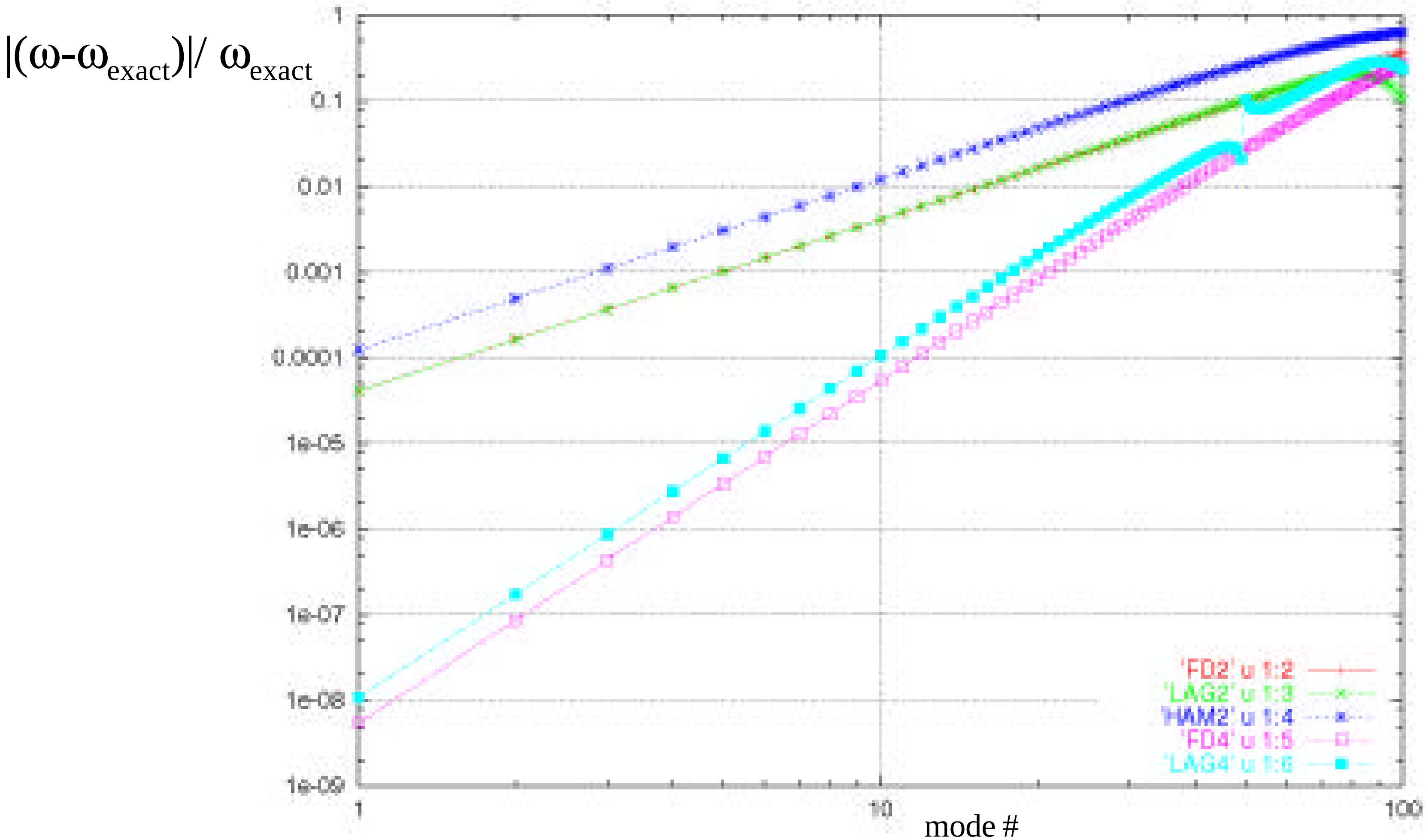
$$H_k = \frac{1}{6r}(p_k^2 + p_k p_{k+1} + p_{k+1}^2) + \frac{T}{2h^2}(u_{k+1} - u_k)^2$$

- Can also be done for quadratic and higher order elements
- Problem: Quadratic case appears to have poor dispersive characteristics, not even the correct behavior for long λ

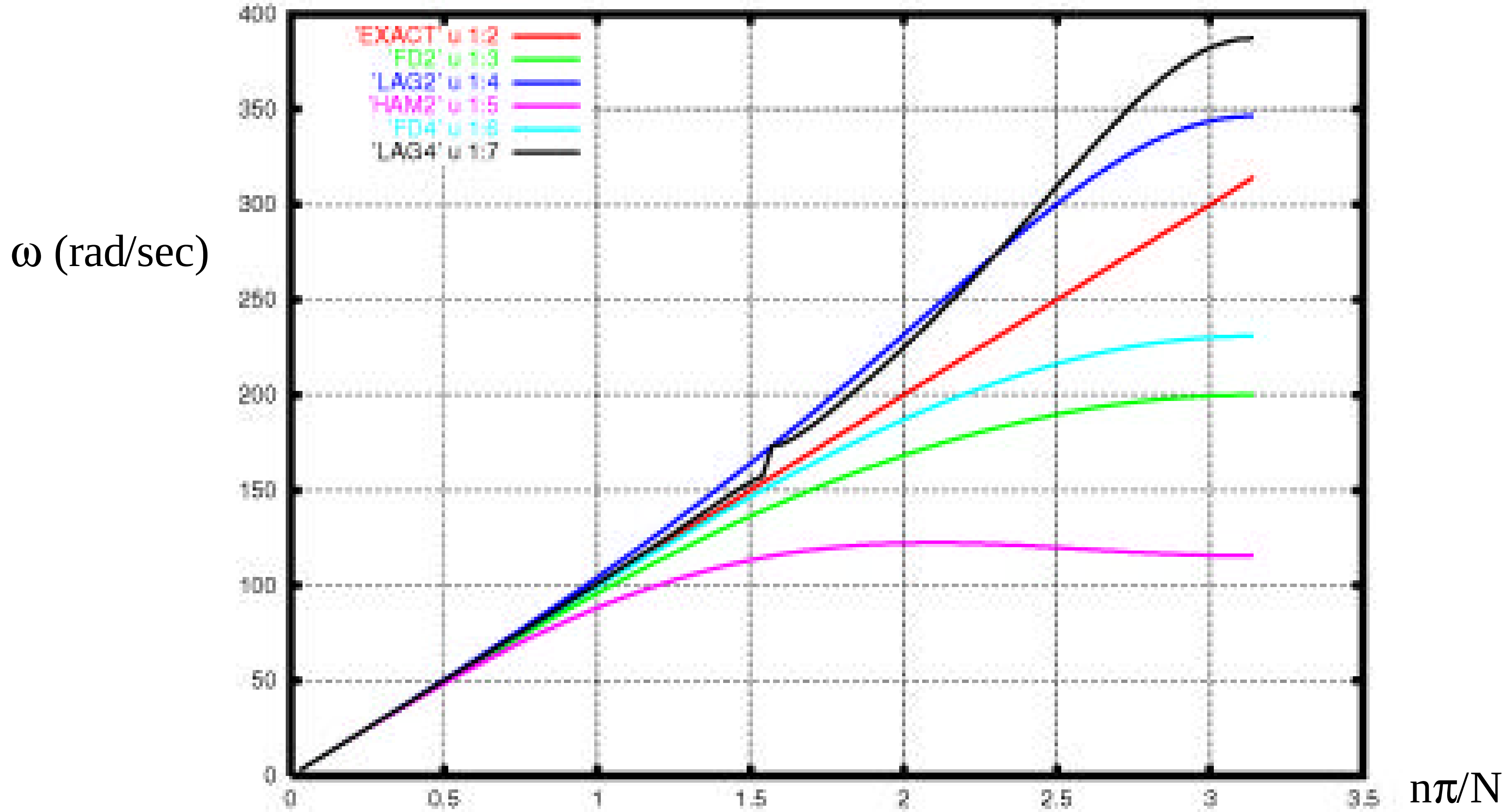
Comparison of Eigenfrequencies



Comparison of Eigenfrequencies (log plot)



Dispersion Curves



Closing Thoughts

- Many possible models… which is "best"?
  - Alternative to FEM would be to construct a model w/ desired properties
    - The discrete eigenvalues should approach eigenvalues of the continuous system as Δx tends to zero.
    - The dispersion curve should be "near" the exact curve
      - Should probably place greater emphasis on accuracy of low freq modes
    - "Best" is a balance of numerical properties and Hamiltonian bandwidth